

n-Caprylic acid isobutyl ester

Other names:	Octanoic acid, 2-methylpropyl ester iso-Butyl caprylate Octanoic acid, isobutyl ester iso-Butyl n-octanoate Isobutyl octanoate 2-Methylpropyl octanoate
Inchi:	InChI=1S/C12H24O2/c1-4-5-6-7-8-9-12(13)14-10-11(2)3/h11H,4-10H2,1-3H3
InchiKey:	CFQRBRGFNFRMBD-UHFFFAOYSA-N
Formula:	C12H24O2
SMILES:	CCCCCCCC(=O)OCC(C)C
Mol. weight [g/mol]:	200.32
CAS:	5461-06-3

Physical Properties

Property code	Value	Unit	Source
gf	-186.20	kJ/mol	Joback Method
hf	-541.09	kJ/mol	Joback Method
hfus	26.10	kJ/mol	Joback Method
hvap	51.07	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	3.546		Crippen Method
mcvol	187.380	ml/mol	McGowan Method
pc	1864.33	kPa	Joback Method
rinpol	1348.00		NIST Webbook
rinpol	1351.00		NIST Webbook
rinpol	1350.00		NIST Webbook
rinpol	1348.00		NIST Webbook
rinpol	1327.00		NIST Webbook
rinpol	1345.00		NIST Webbook
rinpol	1348.00		NIST Webbook
rinpol	1348.10		NIST Webbook
rinpol	1348.00		NIST Webbook
rinpol	1348.00		NIST Webbook
rinpol	1334.00		NIST Webbook
rinpol	1334.00		NIST Webbook
rinpol	1348.00		NIST Webbook
rinpol	1334.00		NIST Webbook

ripol	1338.00		NIST Webbook
ripol	1561.00		NIST Webbook
ripol	1551.00		NIST Webbook
ripol	1550.00		NIST Webbook
ripol	1561.00		NIST Webbook
ripol	1543.00		NIST Webbook
ripol	1550.00		NIST Webbook
ripol	1551.00		NIST Webbook
ripol	1545.00		NIST Webbook
ripol	1537.00		NIST Webbook
ripol	1545.00		NIST Webbook
ripol	1537.00		NIST Webbook
ripol	1551.00		NIST Webbook
ripol	1550.00		NIST Webbook
tb	549.81	K	Joback Method
tc	722.69	K	Joback Method
tf	282.16	K	Joback Method
vc	0.726	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.44	J/molxK	549.81	Joback Method
cpg	480.46	J/molxK	578.62	Joback Method
cpg	495.83	J/molxK	607.44	Joback Method
cpg	510.57	J/molxK	636.25	Joback Method
cpg	524.69	J/molxK	665.07	Joback Method
cpg	538.20	J/molxK	693.88	Joback Method
cpg	551.11	J/molxK	722.69	Joback Method
dvisc	0.0042661	Paxs	282.16	Joback Method
dvisc	0.0017460	Paxs	326.77	Joback Method
dvisc	0.0008857	Paxs	371.38	Joback Method
dvisc	0.0005197	Paxs	415.99	Joback Method
dvisc	0.0003381	Paxs	460.59	Joback Method
dvisc	0.0002373	Paxs	505.20	Joback Method
dvisc	0.0001764	Paxs	549.81	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5461063&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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