n-Capric acid isobutyl ester

Other names:	Decanoic acid, 2-methylpropyl ester
	Decanoic acid, isobutyl ester
	Isobutyl decanoate
	2-Methylpropyl decanoate
	Isobutyl caprate
Inchi:	InChI=1S/C14H28O2/c1-4-5-6-7-8-9-10-11-14(15)16-12-13(2)3/h13H,4-12H2,1-3H3
InchiKey:	AXTPGRJJIGEOOY-UHFFFAOYSA-N
Formula:	C14H28O2
SMILES:	CCCCCCCCCC(=O)OCC(C)C
Mol. weight [g/mol]:	228.37
CAS:	30673-38-2

Physical Properties

Property code	Value	Unit	Source
gf	-169.36	kJ/mol	Joback Method
hf	-582.37	kJ/mol	Joback Method
hfus	31.28	kJ/mol	Joback Method
hvap	55.53	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	4.326		Crippen Method
mcvol	215.560	ml/mol	McGowan Method
pc	1589.81	kPa	Joback Method
rinpol	1528.00		NIST Webbook
rinpol	1528.00		NIST Webbook
rinpol	1545.00		NIST Webbook
rinpol	1545.00		NIST Webbook
rinpol	1533.00		NIST Webbook
rinpol	1574.00		NIST Webbook
rinpol	1550.00		NIST Webbook
rinpol	1549.50		NIST Webbook
rinpol	1546.00		NIST Webbook
rinpol	1545.00		NIST Webbook
rinpol	1549.50		NIST Webbook
ripol	1751.00		NIST Webbook
ripol	1756.00		NIST Webbook
ripol	1750.00		NIST Webbook
ripol	1748.00		NIST Webbook

ripol	1749.00		NIST Webbook
ripol	1756.00		NIST Webbook
ripol	1750.00		NIST Webbook
ripol	1751.00		NIST Webbook
tb	595.57	K	Joback Method
tc	766.26	K	Joback Method
tf	304.70	K	Joback Method
vc	0.838	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	567.35	J/mol×K	595.57	Joback Method
cpg	584.55	J/mol×K	624.02	Joback Method
cpg	601.04	J/mol×K	652.47	Joback Method
cpg	616.82	J/mol×K	680.91	Joback Method
cpg	631.92	J/mol×K	709.36	Joback Method
cpg	646.34	J/mol×K	737.81	Joback Method
cpg	660.10	J/mol×K	766.26	Joback Method
dvisc	0.0037349	Pa×s	304.70	Joback Method
dvisc	0.0014934	Pa×s	353.18	Joback Method
dvisc	0.0007451	Pa×s	401.66	Joback Method
dvisc	0.0004318	Pa×s	450.13	Joback Method
dvisc	0.0002782	Pa×s	498.61	Joback Method
dvisc	0.0001938	Pa×s	547.09	Joback Method
dvisc	0.0001432	Pa×s	595.57	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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=C30673382&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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