

3-Octenoic acid, isobutyl ester

Inchi:	InChI=1S/C12H22O2/c1-4-5-6-7-8-9-12(13)14-10-11(2)3/h7-8,11H,4-6,9-10H2,1-3H3/b8
InchiKey:	BXLSKVVHVVMXOV-BQYQJAHWSA-N
Formula:	C12H22O2
SMILES:	CCCCC=CCC(=O)OCC(C)C
Mol. weight [g/mol]:	198.30

Physical Properties

Property code	Value	Unit	Source
gf	-105.98	kJ/mol	Joback Method
hf	-423.87	kJ/mol	Joback Method
hfus	26.30	kJ/mol	Joback Method
hvap	51.03	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	3.322		Crippen Method
mcvol	183.080	ml/mol	McGowan Method
pc	1950.95	kPa	Joback Method
rinpol	1348.00		NIST Webbook
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tb	553.97	K	Joback Method
tc	733.78	K	Joback Method
tf	277.08	K	Joback Method
vc	0.706	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.03	J/molxK	553.97	Joback Method
cpg	461.70	J/molxK	583.94	Joback Method
cpg	476.67	J/molxK	613.91	Joback Method
cpg	490.97	J/molxK	643.87	Joback Method
cpg	504.62	J/molxK	673.84	Joback Method
cpg	517.63	J/molxK	703.81	Joback Method
cpg	530.02	J/molxK	733.78	Joback Method
dvisc	0.0040101	Paxs	277.08	Joback Method

dvisc	0.0015677	Paxs	323.23	Joback Method
dvisc	0.0007750	Paxs	369.38	Joback Method
dvisc	0.0004480	Paxs	415.52	Joback Method
dvisc	0.0002890	Paxs	461.67	Joback Method
dvisc	0.0002019	Paxs	507.82	Joback Method
dvisc	0.0001497	Paxs	553.97	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U406123&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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