

Butanoic acid, 6-ethyl-3-octyl ester

Inchi:	InChI=1S/C14H28O2/c1-5-9-14(15)16-13(8-4)11-10-12(6-2)7-3/h12-13H,5-11H2,1-4H3
InchiKey:	QTIXZPIDWBOJMH-UHFFFAOYSA-N
Formula:	C14H28O2
SMILES:	CCCC(=O)OC(CC)CCC(CC)CC
Mol. weight [g/mol]:	228.37

Physical Properties

Property code	Value	Unit	Source
gf	-171.80	kJ/mol	Joback Method
hf	-587.65	kJ/mol	Joback Method
hfus	27.76	kJ/mol	Joback Method
hvap	55.14	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	4.325		Crippen Method
mvol	215.560	ml/mol	McGowan Method
pc	1600.00	kPa	Joback Method
rinpol	1190.00		NIST Webbook
rinpol	1190.00		NIST Webbook
tb	595.13	K	Joback Method
tc	768.62	K	Joback Method
tf	289.70	K	Joback Method
vc	0.832	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	567.68	J/molxK	595.13	Joback Method
cpg	648.02	J/molxK	739.70	Joback Method
cpg	633.39	J/molxK	710.79	Joback Method
cpg	618.05	J/molxK	681.87	Joback Method
cpg	602.00	J/molxK	652.96	Joback Method
cpg	585.21	J/molxK	624.04	Joback Method
cpg	661.96	J/molxK	768.62	Joback Method
dvisc	0.0001338	Paxs	595.13	Joback Method

dvisc	0.0001853	Paxs	544.23	Joback Method
dvisc	0.0002745	Paxs	493.32	Joback Method
dvisc	0.0004451	Paxs	442.42	Joback Method
dvisc	0.0008184	Paxs	391.51	Joback Method
dvisc	0.0018054	Paxs	340.61	Joback Method
dvisc	0.0052596	Paxs	289.70	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U282601&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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