

Isovaleric acid, tetradecyl ester

Inchi:	InChI=1S/C19H38O2/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-21-19(20)17-18(2)3/h18H,4-
InchiKey:	LDFVABHBWXREIO-UHFFFAOYSA-N
Formula:	C19H38O2
SMILES:	CCCCCCCCCCCCCOC(=O)CC(C)C
Mol. weight [g/mol]:	298.50

Physical Properties

Property code	Value	Unit	Source
gf	-127.26	kJ/mol	Joback Method
hf	-685.57	kJ/mol	Joback Method
hfus	44.23	kJ/mol	Joback Method
hvap	66.66	kJ/mol	Joback Method
log10ws	-6.40		Crippen Method
logp	6.277		Crippen Method
mvol	286.010	ml/mol	McGowan Method
pc	1120.05	kPa	Joback Method
rinpol	2048.00		NIST Webbook
rinpol	2048.00		NIST Webbook
tb	709.97	K	Joback Method
tc	880.96	K	Joback Method
tf	361.05	K	Joback Method
vc	1.117	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	849.12	J/molxK	709.97	Joback Method
cpg	868.53	J/molxK	738.47	Joback Method
cpg	887.04	J/molxK	766.97	Joback Method
cpg	904.69	J/molxK	795.46	Joback Method
cpg	921.48	J/molxK	823.96	Joback Method
cpg	937.44	J/molxK	852.46	Joback Method
cpg	952.60	J/molxK	880.96	Joback Method
dvisc	0.0023450	Paxs	361.05	Joback Method

dvisc	0.0008954	Paxs	419.20	Joback Method
dvisc	0.0004323	Paxs	477.36	Joback Method
dvisc	0.0002445	Paxs	535.51	Joback Method
dvisc	0.0001546	Paxs	593.66	Joback Method
dvisc	0.0001061	Paxs	651.82	Joback Method
dvisc	0.0000774	Paxs	709.97	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=U340262&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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