

Isovaleric acid, pentadecyl ester

Inchi:	InChI=1S/C20H40O2/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-22-20(21)18-19(2)3/h19H
InchiKey:	NJOJSCYAQJIGHN-UHFFFAOYSA-N
Formula:	C20H40O2
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CC(C)C
Mol. weight [g/mol]:	312.53

Physical Properties

Property code	Value	Unit	Source
gf	-118.84	kJ/mol	Joback Method
hf	-706.21	kJ/mol	Joback Method
hfus	46.82	kJ/mol	Joback Method
hvap	68.88	kJ/mol	Joback Method
log10ws	-6.82		Crippen Method
logp	6.667		Crippen Method
mvol	300.100	ml/mol	McGowan Method
pc	1051.41	kPa	Joback Method
rinpol	2138.00		NIST Webbook
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tb	732.85	K	Joback Method
tc	905.32	K	Joback Method
tf	372.32	K	Joback Method
vc	1.173	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	908.95	J/molxK	732.85	Joback Method
cpg	998.90	J/molxK	876.57	Joback Method
cpg	982.69	J/molxK	847.83	Joback Method
cpg	965.61	J/molxK	819.08	Joback Method
cpg	947.65	J/molxK	790.34	Joback Method
cpg	928.77	J/molxK	761.59	Joback Method
cpg	1014.26	J/molxK	905.32	Joback Method
dvisc	0.0000677	Paxs	732.85	Joback Method

dvisc	0.0000929	Paxs	672.76	Joback Method
dvisc	0.0001357	Paxs	612.67	Joback Method
dvisc	0.0002153	Paxs	552.59	Joback Method
dvisc	0.0003822	Paxs	492.50	Joback Method
dvisc	0.0007959	Paxs	432.41	Joback Method
dvisc	0.0021002	Paxs	372.32	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U340263&Units=SI
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

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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