

Isovaleric acid, heptadecyl ester

Inchi:	InChI=1S/C22H44O2/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-24-22(23)20-21(2)
InchiKey:	PRIFMYWTZKZMDP-UHFFFAOYSA-N
Formula:	C22H44O2
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CC(C)C
Mol. weight [g/mol]:	340.58

Physical Properties

Property code	Value	Unit	Source
gf	-102.00	kJ/mol	Joback Method
hf	-747.49	kJ/mol	Joback Method
hfus	52.00	kJ/mol	Joback Method
hvap	73.33	kJ/mol	Joback Method
log10ws	-7.65		Crippen Method
logp	7.447		Crippen Method
mcvol	328.280	ml/mol	McGowan Method
pc	931.78	kPa	Joback Method
rinpol	2344.00		NIST Webbook
rinpol	2344.00		NIST Webbook
tb	778.61	K	Joback Method
tc	955.90	K	Joback Method
tf	394.86	K	Joback Method
vc	1.286	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1031.45	J/molxK	778.61	Joback Method
cpg	1052.12	J/molxK	808.16	Joback Method
cpg	1071.76	J/molxK	837.71	Joback Method
cpg	1090.39	J/molxK	867.25	Joback Method
cpg	1108.04	J/molxK	896.80	Joback Method
cpg	1124.73	J/molxK	926.35	Joback Method
cpg	1140.50	J/molxK	955.90	Joback Method
dvisc	0.0016625	Paxs	394.86	Joback Method

dvisc	0.0006213	Paxs	458.82	Joback Method
dvisc	0.0002954	Paxs	522.78	Joback Method
dvisc	0.0001652	Paxs	586.74	Joback Method
dvisc	0.0001035	Paxs	650.69	Joback Method
dvisc	0.0000706	Paxs	714.65	Joback Method
dvisc	0.0000512	Paxs	778.61	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=U340265&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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