

Pimelic acid, isobutyl 1-methoxydec-4-yl ester

Inchi:	InChI=1S/C22H42O5/c1-5-6-7-9-13-20(14-12-17-25-4)27-22(24)16-11-8-10-15-21(23)26
InchiKey:	SWFYFYNLFAINCF-UHFFFAOYSA-N
Formula:	C22H42O5
SMILES:	CCCCCCC(CCCOC)OC(=O)CCCCC(=O)OCC(C)C
Mol. weight [g/mol]:	386.57

Physical Properties

Property code	Value	Unit	Source
gf	-443.36	kJ/mol	Joback Method
hf	-1129.79	kJ/mol	Joback Method
hfus	52.45	kJ/mol	Joback Method
hvap	84.51	kJ/mol	Joback Method
log10ws	-5.71		Crippen Method
logp	5.445		Crippen Method
mvol	341.590	ml/mol	McGowan Method
pc	953.19	kPa	Joback Method
rinpol	2467.00		NIST Webbook
rinpol	2467.00		NIST Webbook
tb	876.88	K	Joback Method
tc	1073.55	K	Joback Method
tf	474.25	K	Joback Method
vc	1.321	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1125.01	J/molxK	876.88	Joback Method
cpg	1206.02	J/molxK	1040.78	Joback Method
cpg	1192.45	J/molxK	1008.00	Joback Method
cpg	1177.58	J/molxK	975.22	Joback Method
cpg	1161.39	J/molxK	942.44	Joback Method
cpg	1143.87	J/molxK	909.66	Joback Method
cpg	1218.30	J/molxK	1073.55	Joback Method
dvisc	0.0000247	Paxs	876.88	Joback Method

dvisc	0.0000338	Paxs	809.78	Joback Method
dvisc	0.0000489	Paxs	742.67	Joback Method
dvisc	0.0000762	Paxs	675.57	Joback Method
dvisc	0.0001310	Paxs	608.46	Joback Method
dvisc	0.0002574	Paxs	541.36	Joback Method
dvisc	0.0006124	Paxs	474.25	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=U406768&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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