

Pimelic acid, undecyl 3-methylbutyl ester

Inchi: InChI=1S/C23H44O4/c1-4-5-6-7-8-9-10-11-15-19-26-22(24)16-13-12-14-17-23(25)27-20
InchiKey: YXCYGKXCKWSWFH-UHFFFAOYSA-N
Formula: C23H44O4
SMILES: CCCCCCCCCCOC(=O)CCCCC(=O)OCCC(C)C
Mol. weight [g/mol]: 384.59

Physical Properties

Property code	Value	Unit	Source
gf	-327.50	kJ/mol	Joback Method
hf	-1012.93	kJ/mol	Joback Method
hfus	57.38	kJ/mol	Joback Method
hvap	84.72	kJ/mol	Joback Method
log10ws	-6.93		Crippen Method
logp	6.600		Crippen Method
mvol	349.810	ml/mol	McGowan Method
pc	903.97	kPa	Joback Method
rinpol	2628.00		NIST Webbook
rinpol	2628.00		NIST Webbook
tb	877.78	K	Joback Method
tc	1074.72	K	Joback Method
tf	478.29	K	Joback Method
vc	1.365	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1154.96	J/molxK	877.78	Joback Method
cpg	1174.58	J/molxK	910.60	Joback Method
cpg	1192.90	J/molxK	943.43	Joback Method
cpg	1209.94	J/molxK	976.25	Joback Method
cpg	1225.74	J/molxK	1009.07	Joback Method
cpg	1240.32	J/molxK	1041.89	Joback Method
cpg	1253.72	J/molxK	1074.72	Joback Method
dvisc	0.0006901	Paxs	478.29	Joback Method

dvisc	0.0003008	Paxs	544.87	Joback Method
dvisc	0.0001571	Paxs	611.45	Joback Method
dvisc	0.0000932	Paxs	678.03	Joback Method
dvisc	0.0000607	Paxs	744.62	Joback Method
dvisc	0.0000424	Paxs	811.20	Joback Method
dvisc	0.0000313	Paxs	877.78	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=U393779&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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