

Pimelic acid, heptyl 3-(2-methoxyethyl)heptyl ester

Inchi:	InChI=1S/C24H46O5/c1-4-6-8-9-13-19-28-23(25)15-11-10-12-16-24(26)29-21-18-22(14-
InchiKey:	NZLVSFYAOWHWHM-UHFFFAOYSA-N
Formula:	C24H46O5
SMILES:	CCCCCCCOC(=O)CCCCC(=O)OCCC(CCCC)CCOC
Mol. weight [g/mol]:	414.62

Physical Properties

Property code	Value	Unit	Source
gf	-424.08	kJ/mol	Joback Method
hf	-1165.79	kJ/mol	Joback Method
hfus	61.16	kJ/mol	Joback Method
hvap	89.35	kJ/mol	Joback Method
log10ws	-6.44		Crippen Method
logp	6.227		Crippen Method
mcvol	369.770	ml/mol	McGowan Method
pc	845.54	kPa	Joback Method
rinpol	2756.00		NIST Webbook
rinpol	2756.00		NIST Webbook
tb	923.08	K	Joback Method
tc	1132.65	K	Joback Method
tf	511.79	K	Joback Method
vc	1.440	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1250.13	J/molxK	923.08	Joback Method
cpg	1269.91	J/molxK	958.01	Joback Method
cpg	1288.10	J/molxK	992.94	Joback Method
cpg	1304.72	J/molxK	1027.86	Joback Method
cpg	1319.81	J/molxK	1062.79	Joback Method
cpg	1333.37	J/molxK	1097.72	Joback Method
cpg	1345.43	J/molxK	1132.65	Joback Method
dvisc	0.0004053	Paxs	511.79	Joback Method

dvisc	0.0001821	Paxs	580.34	Joback Method
dvisc	0.0000969	Paxs	648.89	Joback Method
dvisc	0.0000582	Paxs	717.43	Joback Method
dvisc	0.0000382	Paxs	785.98	Joback Method
dvisc	0.0000268	Paxs	854.53	Joback Method
dvisc	0.0000198	Paxs	923.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406786&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

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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