

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

Inchi:	InChI=1S/C27H52O6/c1-5-7-10-14-24(18-20-30-3)22-32-26(28)16-12-9-13-17-27(29)33-
InchiKey:	ICEMGFSATXUTGS-UHFFFAOYSA-N
Formula:	C27H52O6
SMILES:	CCCCC(CCOC)COC(=O)CCCCC(=O)OCC(CCCCC)CCOC
Mol. weight [g/mol]:	472.70

Physical Properties

Property code	Value	Unit	Source
gf	-506.26	kJ/mol	Joback Method
hf	-1365.21	kJ/mol	Joback Method
hfus	66.59	kJ/mol	Joback Method
hvap	98.05	kJ/mol	Joback Method
log10ws	-6.54		Crippen Method
logp	6.489		Crippen Method
mvol	417.910	ml/mol	McGowan Method
pc	716.45	kPa	Joback Method
rinpol	3036.00		NIST Webbook
rinpol	3036.00		NIST Webbook
tb	1013.70	K	Joback Method
tc	1259.37	K	Joback Method
tf	552.83	K	Joback Method
vc	1.619	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1472.76	J/molxK	1013.70	Joback Method
cpg	1493.07	J/molxK	1054.65	Joback Method
cpg	1510.89	J/molxK	1095.59	Joback Method
cpg	1526.25	J/molxK	1136.54	Joback Method
cpg	1539.18	J/molxK	1177.48	Joback Method
cpg	1549.70	J/molxK	1218.43	Joback Method
cpg	1557.86	J/molxK	1259.37	Joback Method
dvisc	0.0002036	Paxs	552.83	Joback Method

dvisc	0.0000859	Paxs	629.64	Joback Method
dvisc	0.0000437	Paxs	706.45	Joback Method
dvisc	0.0000254	Paxs	783.26	Joback Method
dvisc	0.0000163	Paxs	860.08	Joback Method
dvisc	0.0000112	Paxs	936.89	Joback Method
dvisc	0.0000082	Paxs	1013.70	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=U406741&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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