

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

Inchi:	InChI=1S/C26H50O5/c1-4-6-8-10-15-21-30-25(27)17-13-11-14-18-26(28)31-23-20-24(19)
InchiKey:	BLIIUEQHBBZSAM-UHFFFAOYSA-N
Formula:	C26H50O5
SMILES:	CCCCCCCOC(=O)CCCCC(=O)OCCC(CCCCC)CCOC
Mol. weight [g/mol]:	442.67

Physical Properties

Property code	Value	Unit	Source
gf	-407.24	kJ/mol	Joback Method
hf	-1207.07	kJ/mol	Joback Method
hfus	66.33	kJ/mol	Joback Method
hvap	93.80	kJ/mol	Joback Method
log10ws	-7.28		Crippen Method
logp	7.007		Crippen Method
mcvol	397.950	ml/mol	McGowan Method
pc	758.49	kPa	Joback Method
rinpol	2940.00		NIST Webbook
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tb	968.84	K	Joback Method
tc	1195.64	K	Joback Method
tf	534.33	K	Joback Method
vc	1.552	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1377.50	J/molxK	968.84	Joback Method
cpg	1398.28	J/molxK	1006.64	Joback Method
cpg	1417.13	J/molxK	1044.44	Joback Method
cpg	1434.09	J/molxK	1082.24	Joback Method
cpg	1449.19	J/molxK	1120.04	Joback Method
cpg	1462.47	J/molxK	1157.84	Joback Method
cpg	1473.97	J/molxK	1195.64	Joback Method
dvisc	0.0003107	Paxs	534.33	Joback Method

dvisc	0.0001373	Paxs	606.75	Joback Method
dvisc	0.0000722	Paxs	679.17	Joback Method
dvisc	0.0000430	Paxs	751.58	Joback Method
dvisc	0.0000281	Paxs	824.00	Joback Method
dvisc	0.0000196	Paxs	896.42	Joback Method
dvisc	0.0000145	Paxs	968.84	Joback Method

Sources

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=U406761&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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