

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

Inchi:	InChI=1S/C19H36O5/c1-4-6-10-17(13-15-22-3)14-16-24-19(21)12-9-7-8-11-18(20)23-5-2
InchiKey:	AGYWDMSPJSOAIZ-UHFFFAOYSA-N
Formula:	C19H36O5
SMILES:	CCCCC(CCOC)CCOC(=O)CCCCC(=O)OCC
Mol. weight [g/mol]:	344.49

Physical Properties

Property code	Value	Unit	Source
gf	-466.18	kJ/mol	Joback Method
hf	-1062.59	kJ/mol	Joback Method
hfus	48.20	kJ/mol	Joback Method
hvap	78.22	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	4.276		Crippen Method
mvol	299.320	ml/mol	McGowan Method
pc	1142.12	kPa	Joback Method
rinpol	2282.00		NIST Webbook
rinpol	2282.00		NIST Webbook
tb	808.68	K	Joback Method
tc	993.30	K	Joback Method
tf	455.44	K	Joback Method
vc	1.159	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	940.75	J/molxK	808.68	Joback Method
cpg	958.44	J/molxK	839.45	Joback Method
cpg	975.07	J/molxK	870.22	Joback Method
cpg	990.65	J/molxK	900.99	Joback Method
cpg	1005.16	J/molxK	931.76	Joback Method
cpg	1018.64	J/molxK	962.53	Joback Method
cpg	1031.06	J/molxK	993.30	Joback Method
dvisc	0.0007490	Paxs	455.44	Joback Method

dvisc	0.0003527	Paxs	514.31	Joback Method
dvisc	0.0001939	Paxs	573.19	Joback Method
dvisc	0.0001192	Paxs	632.06	Joback Method
dvisc	0.0000796	Paxs	690.93	Joback Method
dvisc	0.0000566	Paxs	749.81	Joback Method
dvisc	0.0000423	Paxs	808.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406779&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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