

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

Inchi:	InChI=1S/C23H44O5/c1-4-6-8-10-13-21(16-19-26-3)17-20-28-23(25)15-12-9-11-14-22(2
InchiKey:	TVNFPUISDZYQGG-UHFFFAOYSA-N
Formula:	C23H44O5
SMILES:	CCCCCCC(CCOC)CCOC(=O)CCCCC(=O)OCCCC
Mol. weight [g/mol]:	400.59

Physical Properties

Property code	Value	Unit	Source
gf	-432.50	kJ/mol	Joback Method
hf	-1145.15	kJ/mol	Joback Method
hfus	58.56	kJ/mol	Joback Method
hvap	87.13	kJ/mol	Joback Method
log10ws	-6.02		Crippen Method
logp	5.837		Crippen Method
mcvol	355.680	ml/mol	McGowan Method
pc	894.80	kPa	Joback Method
rinpol	2648.00		NIST Webbook
rinpol	2648.00		NIST Webbook
tb	900.20	K	Joback Method
tc	1102.87	K	Joback Method
tf	500.52	K	Joback Method
vc	1.383	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1187.09	J/molxK	900.20	Joback Method
cpg	1206.41	J/molxK	933.98	Joback Method
cpg	1224.28	J/molxK	967.76	Joback Method
cpg	1240.71	J/molxK	1001.53	Joback Method
cpg	1255.73	J/molxK	1035.31	Joback Method
cpg	1269.34	J/molxK	1069.09	Joback Method
cpg	1281.58	J/molxK	1102.87	Joback Method
dvisc	0.0004611	Paxs	500.52	Joback Method

dvisc	0.0002090	Paxs	567.13	Joback Method
dvisc	0.0001118	Paxs	633.75	Joback Method
dvisc	0.0000674	Paxs	700.36	Joback Method
dvisc	0.0000444	Paxs	766.97	Joback Method
dvisc	0.0000312	Paxs	833.59	Joback Method
dvisc	0.0000231	Paxs	900.20	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=U406757&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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