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

Inchi: InChI=1S/C20H38O5/c1-4-6-10-18(13-16-23-3)14-17-25-20(22)12-9-7-8-11-19(21)24-15

InchiKey: UGOSNAIIVKONPZ-UHFFFAOYSA-N

Formula: C20H38O5

SMILES: CCCCC(CCOC)CCOC(=O)CCCCCC(=O)OCCC

Mol. weight [g/mol]: 358.51

Physical Properties

Property code	Value	Unit	Source
gf	-457.76	kJ/mol	Joback Method
hf	-1083.23	kJ/mol	Joback Method
hfus	50.80	kJ/mol	Joback Method
hvap	80.45	kJ/mol	Joback Method
log10ws	-4.77		Crippen Method
logp	4.666		Crippen Method
mcvol	313.410	ml/mol	McGowan Method
pc	1071.46	kPa	Joback Method
rinpol	2377.00		NIST Webbook
rinpol	2377.00		NIST Webbook
tb	831.56	K	Joback Method
tc	1019.41	K	Joback Method
tf	466.71	K	Joback Method
vc	1.216	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1001.32	J/mol×K	831.56	Joback Method
cpg	1019.40	J/mol×K	862.87	Joback Method
cpg	1036.34	J/mol×K	894.18	Joback Method
cpg	1052.14	J/mol×K	925.48	Joback Method
cpg	1066.81	J/mol×K	956.79	Joback Method
cpg	1080.36	J/mol×K	988.10	Joback Method
cpg	1092.80	J/mol×K	1019.41	Joback Method
dvisc	0.0006668	Pa×s	466.71	Joback Method

dvisc	0.0003109	Pa×s	527.52	Joback Method
dvisc	0.0001697	Pa×s	588.33	Joback Method
dvisc	0.0001037	Pa×s	649.13	Joback Method
dvisc	0.0000690	Pa×s	709.94	Joback Method
dvisc	0.0000489	Pa×s	770.75	Joback Method
dvisc	0.0000365	Pa×s	831.56	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406780&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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