Pimelic acid, di(octyl) ester

Other names: Dioctyl pimelate
Inchi: InChI=1S/C23H44O4/c1-3-5-7-9-11-16-20-26-22(24)18-14-13-15-19-23(25)27-21-17-12-
InchiKey: MADOOBPQEFYJRB-UHFFFAOYSA-N
Formula: C23H44O4
SMILES: CCCCCCCCOC(=O)CCCCCC(=O)OCCCCCCCC
Mol. weight [g/mol]: 384.59

Physical Properties

Property code	Value	Unit	Source
gf	-325.06	kJ/mol	Joback Method
hf	-1007.65	kJ/mol	Joback Method
hfus	60.90	kJ/mol	Joback Method
hvap	85.10	kJ/mol	Joback Method
log10ws	-7.18		Crippen Method
logp	6.744		Crippen Method
mcvol	349.810	ml/mol	McGowan Method
pc	899.64	kPa	Joback Method
rinpol	2684.00		NIST Webbook
rinpol	2599.00		NIST Webbook
rinpol	2684.00		NIST Webbook
rinpol	2599.00		NIST Webbook
tb	878.22	K	Joback Method
tc	1075.46	K	Joback Method
tf	493.29	K	Joback Method
vc	1.371	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1154.52	J/mol×K	878.22	Joback Method
cpg	1174.19	J/mol×K	911.09	Joback Method
cpg	1192.56	J/mol×K	943.97	Joback Method
cpg	1209.66	J/mol×K	976.84	Joback Method
cpg	1225.52	J/mol×K	1009.71	Joback Method

cpg	1240.17	J/mol×K	1042.59	Joback Method
cpg	1253.64	J/mol×K	1075.46	Joback Method
dvisc	0.0005944	Pa×s	493.29	Joback Method
dvisc	0.0002809	Pa×s	557.44	Joback Method
dvisc	0.0001550	Pa×s	621.60	Joback Method
dvisc	0.0000955	Pa×s	685.75	Joback Method
dvisc	0.0000640	Pa×s	749.91	Joback Method
dvisc	0.0000457	Pa×s	814.07	Joback Method
dvisc	0.0000342	Pa×s	878.22	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=U393881&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