

Pimelic acid, 2-methylpentyl octyl ester

Inchi:	InChI=1S/C21H40O4/c1-4-6-7-8-9-13-17-24-20(22)15-11-10-12-16-21(23)25-18-19(3)14
InchiKey:	ZVSLDTCRFYDSDQ-UHFFFAOYSA-N
Formula:	C21H40O4
SMILES:	CCCCCCCCOC(=O)CCCCC(=O)OCC(C)CCC
Mol. weight [g/mol]:	356.54

Physical Properties

Property code	Value	Unit	Source
gf	-344.34	kJ/mol	Joback Method
hf	-971.65	kJ/mol	Joback Method
hfus	52.20	kJ/mol	Joback Method
hvap	80.26	kJ/mol	Joback Method
log10ws	-6.10		Crippen Method
logp	5.820		Crippen Method
mvol	321.630	ml/mol	McGowan Method
pc	1018.13	kPa	Joback Method
rinpol	2405.00		NIST Webbook
rinpol	2405.00		NIST Webbook
tb	832.02	K	Joback Method
tc	1019.80	K	Joback Method
tf	455.75	K	Joback Method
vc	1.254	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1030.73	J/molxK	832.02	Joback Method
cpg	1049.46	J/molxK	863.32	Joback Method
cpg	1067.07	J/molxK	894.61	Joback Method
cpg	1083.56	J/molxK	925.91	Joback Method
cpg	1098.97	J/molxK	957.21	Joback Method
cpg	1113.31	J/molxK	988.51	Joback Method
cpg	1126.61	J/molxK	1019.80	Joback Method
dvisc	0.0008818	Paxs	455.75	Joback Method

dvisc	0.0003912	Paxs	518.46	Joback Method
dvisc	0.0002068	Paxs	581.17	Joback Method
dvisc	0.0001238	Paxs	643.88	Joback Method
dvisc	0.0000812	Paxs	706.60	Joback Method
dvisc	0.0000570	Paxs	769.31	Joback Method
dvisc	0.0000422	Paxs	832.02	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=U406669&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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