

Pimelic acid, hexyl 2,4,4-trimethylpentyl ester

Inchi:	InChI=1S/C21H40O4/c1-6-7-8-12-15-24-19(22)13-10-9-11-14-20(23)25-17-18(2)16-21(3)
InchiKey:	RFBLQTYYPIDJQ-UHFFFAOYSA-N
Formula:	C21H40O4
SMILES:	CCCCCOC(=O)CCCCC(=O)OCC(C)CC(C)(C)C
Mol. weight [g/mol]:	356.54

Physical Properties

Property code	Value	Unit	Source
gf	-341.50	kJ/mol	Joback Method
hf	-980.40	kJ/mol	Joback Method
hfus	44.78	kJ/mol	Joback Method
hvap	78.97	kJ/mol	Joback Method
log10ws	-5.85		Crippen Method
logp	5.676		Crippen Method
mvol	321.630	ml/mol	McGowan Method
pc	1030.59	kPa	Joback Method
rinpol	1737.00		NIST Webbook
rinpol	1737.00		NIST Webbook
tb	828.79	K	Joback Method
tc	1018.11	K	Joback Method
tf	458.17	K	Joback Method
vc	1.242	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1031.48	J/molxK	828.79	Joback Method
cpg	1050.15	J/molxK	860.34	Joback Method
cpg	1067.69	J/molxK	891.90	Joback Method
cpg	1084.15	J/molxK	923.45	Joback Method
cpg	1099.56	J/molxK	955.00	Joback Method
cpg	1113.95	J/molxK	986.55	Joback Method
cpg	1127.36	J/molxK	1018.11	Joback Method
dvisc	0.0008434	Paxs	458.17	Joback Method

dvisc	0.0003582	Paxs	519.94	Joback Method
dvisc	0.0001825	Paxs	581.71	Joback Method
dvisc	0.0001058	Paxs	643.48	Joback Method
dvisc	0.0000675	Paxs	705.25	Joback Method
dvisc	0.0000463	Paxs	767.02	Joback Method
dvisc	0.0000336	Paxs	828.79	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=U406474&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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