

Pimelic acid, hexyl 3-methylbutyl ester

Inchi:	InChI=1S/C18H34O4/c1-4-5-6-10-14-21-17(19)11-8-7-9-12-18(20)22-15-13-16(2)3/h16H
InchiKey:	VPTVALCLVMQPBH-UHFFFAOYSA-N
Formula:	C18H34O4
SMILES:	CCCCCOC(=O)CCCCC(=O)OCCC(C)C
Mol. weight [g/mol]:	314.46

Physical Properties

Property code	Value	Unit	Source
gf	-369.60	kJ/mol	Joback Method
hf	-909.73	kJ/mol	Joback Method
hfus	44.43	kJ/mol	Joback Method
hvap	73.59	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	4.650		Crippen Method
mcvol	279.360	ml/mol	McGowan Method
pc	1234.61	kPa	Joback Method
rinpol	2135.00		NIST Webbook
rinpol	2135.00		NIST Webbook
tb	763.38	K	Joback Method
tc	943.41	K	Joback Method
tf	421.94	K	Joback Method
vc	1.085	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	849.98	J/molxK	763.38	Joback Method
cpg	867.53	J/molxK	793.39	Joback Method
cpg	884.14	J/molxK	823.39	Joback Method
cpg	899.82	J/molxK	853.40	Joback Method
cpg	914.60	J/molxK	883.40	Joback Method
cpg	928.46	J/molxK	913.41	Joback Method
cpg	941.44	J/molxK	943.41	Joback Method
dvisc	0.0012393	Paxs	421.94	Joback Method

dvisc	0.0005664	Paxs	478.85	Joback Method
dvisc	0.0003058	Paxs	535.75	Joback Method
dvisc	0.0001858	Paxs	592.66	Joback Method
dvisc	0.0001232	Paxs	649.57	Joback Method
dvisc	0.0000873	Paxs	706.47	Joback Method
dvisc	0.0000651	Paxs	763.38	Joback Method

Sources

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=U393774&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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