

Pimelic acid, hexyl 5-methoxy-3-methylpent-2-yl ester

Inchi:	InChI=1S/C20H38O5/c1-5-6-7-11-15-24-19(21)12-9-8-10-13-20(22)25-18(3)17(2)14-16-2
InchiKey:	IRQBZAAGFJFHRW-UHFFFAOYSA-N
Formula:	C20H38O5
SMILES:	CCCCCOC(=O)CCCCC(=O)OC(C)C(C)CCOC
Mol. weight [g/mol]:	358.51

Physical Properties

Property code	Value	Unit	Source
gf	-460.20	kJ/mol	Joback Method
hf	-1088.51	kJ/mol	Joback Method
hfus	47.27	kJ/mol	Joback Method
hvap	80.06	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	4.665		Crippen Method
mvol	313.410	ml/mol	McGowan Method
pc	1077.10	kPa	Joback Method
rinpol	2357.00		NIST Webbook
rinpol	2357.00		NIST Webbook
tb	831.12	K	Joback Method
tc	1019.53	K	Joback Method
tf	451.71	K	Joback Method
vc	1.210	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1001.80	J/molxK	831.12	Joback Method
cpg	1019.93	J/molxK	862.52	Joback Method
cpg	1036.90	J/molxK	893.92	Joback Method
cpg	1052.72	J/molxK	925.33	Joback Method
cpg	1067.40	J/molxK	956.73	Joback Method
cpg	1080.94	J/molxK	988.13	Joback Method
cpg	1093.35	J/molxK	1019.53	Joback Method
dvisc	0.0007901	Paxs	451.71	Joback Method

dvisc	0.0003376	Paxs	514.95	Joback Method
dvisc	0.0001737	Paxs	578.18	Joback Method
dvisc	0.0001019	Paxs	641.41	Joback Method
dvisc	0.0000658	Paxs	704.65	Joback Method
dvisc	0.0000456	Paxs	767.88	Joback Method
dvisc	0.0000335	Paxs	831.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406720&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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