

Pimelic acid, hexadecyl 2-pentyl ester

Inchi:	InChI=1S/C28H54O4/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-21-25-31-27(29)23-19-18-2
InchiKey:	ISYMBXHOKPTFFF-UHFFFAOYSA-N
Formula:	C28H54O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CCCCC(=O)OC(C)CCC
Mol. weight [g/mol]:	454.73

Physical Properties

Property code	Value	Unit	Source
gf	-285.40	kJ/mol	Joback Method
hf	-1116.13	kJ/mol	Joback Method
hfus	70.33	kJ/mol	Joback Method
hvap	95.85	kJ/mol	Joback Method
log10ws	-9.38		Crippen Method
logp	8.693		Crippen Method
mvol	420.260	ml/mol	McGowan Method
pc	690.34	kPa	Joback Method
rinpol	3078.00		NIST Webbook
rinpol	3078.00		NIST Webbook
tb	992.18	K	Joback Method
tc	1230.25	K	Joback Method
tf	534.64	K	Joback Method
vc	1.645	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1474.86	J/molxK	992.18	Joback Method
cpg	1567.75	J/molxK	1190.58	Joback Method
cpg	1552.94	J/molxK	1150.90	Joback Method
cpg	1536.31	J/molxK	1111.22	Joback Method
cpg	1517.80	J/molxK	1071.54	Joback Method
cpg	1497.34	J/molxK	1031.86	Joback Method
cpg	1580.84	J/molxK	1230.25	Joback Method
dvisc	0.0000144	Paxs	992.18	Joback Method

dvisc	0.0000196	Paxs	915.92	Joback Method
dvisc	0.0000284	Paxs	839.67	Joback Method
dvisc	0.0000442	Paxs	763.41	Joback Method
dvisc	0.0000759	Paxs	687.15	Joback Method
dvisc	0.0001491	Paxs	610.90	Joback Method
dvisc	0.0003555	Paxs	534.64	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393802&Units=SI
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

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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