

Pimelic acid, hexadecyl pentyl ester

Inchi:	InChI=1S/C28H54O4/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-22-26-32-28(30)24-20-18-1
InchiKey:	XZBAHFSBOZISOM-UHFFFAOYSA-N
Formula:	C28H54O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CCCCC(=O)OCCCCC
Mol. weight [g/mol]:	454.73

Physical Properties

Property code	Value	Unit	Source
gf	-282.96	kJ/mol	Joback Method
hf	-1110.85	kJ/mol	Joback Method
hfus	73.85	kJ/mol	Joback Method
hvap	96.23	kJ/mol	Joback Method
log10ws	-9.27		Crippen Method
logp	8.695		Crippen Method
mvol	420.260	ml/mol	McGowan Method
pc	687.45	kPa	Joback Method
rinpol	3169.00		NIST Webbook
rinpol	3169.00		NIST Webbook
tb	992.62	K	Joback Method
tc	1233.15	K	Joback Method
tf	549.64	K	Joback Method
vc	1.651	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1474.57	J/molxK	992.62	Joback Method
cpg	1497.33	J/molxK	1032.71	Joback Method
cpg	1518.05	J/molxK	1072.80	Joback Method
cpg	1536.79	J/molxK	1112.88	Joback Method
cpg	1553.63	J/molxK	1152.97	Joback Method
cpg	1568.65	J/molxK	1193.06	Joback Method
cpg	1581.91	J/molxK	1233.15	Joback Method
dvisc	0.0003138	Paxs	549.64	Joback Method

dvisc	0.0001419	Paxs	623.47	Joback Method
dvisc	0.0000759	Paxs	697.30	Joback Method
dvisc	0.0000458	Paxs	771.13	Joback Method
dvisc	0.0000302	Paxs	844.96	Joback Method
dvisc	0.0000212	Paxs	918.79	Joback Method
dvisc	0.0000158	Paxs	992.62	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=U393821&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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