

Pimelic acid, 2-methylpentyl tridecyl ester

Inchi: InChI=1S/C26H50O4/c1-4-6-7-8-9-10-11-12-13-14-18-22-29-25(27)20-16-15-17-21-26(2)
InchiKey: YIZSHIKVOOYABP-UHFFFAOYSA-N
Formula: C26H50O4
SMILES: CCCCCCCCCCCCCOC(=O)CCCCC(=O)OCC(C)CCC
Mol. weight [g/mol]: 426.67

Physical Properties

Property code	Value	Unit	Source
gf	-302.24	kJ/mol	Joback Method
hf	-1074.85	kJ/mol	Joback Method
hfus	65.15	kJ/mol	Joback Method
hvap	91.39	kJ/mol	Joback Method
log10ws	-8.19		Crippen Method
logp	7.771		Crippen Method
mvol	392.080	ml/mol	McGowan Method
pc	765.64	kPa	Joback Method
rinpol	2903.00		NIST Webbook
rinpol	2903.00		NIST Webbook
tb	946.42	K	Joback Method
tc	1164.49	K	Joback Method
tf	512.10	K	Joback Method
vc	1.534	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1345.59	J/molxK	946.42	Joback Method
cpg	1435.40	J/molxK	1128.14	Joback Method
cpg	1420.58	J/molxK	1091.80	Joback Method
cpg	1404.25	J/molxK	1055.45	Joback Method
cpg	1386.34	J/molxK	1019.11	Joback Method
cpg	1366.80	J/molxK	982.76	Joback Method
cpg	1448.73	J/molxK	1164.49	Joback Method
dvisc	0.0000197	Paxs	946.42	Joback Method

dvisc	0.0000268	Paxs	874.03	Joback Method
dvisc	0.0000387	Paxs	801.65	Joback Method
dvisc	0.0000599	Paxs	729.26	Joback Method
dvisc	0.0001021	Paxs	656.87	Joback Method
dvisc	0.0001988	Paxs	584.49	Joback Method
dvisc	0.0004671	Paxs	512.10	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=U406674&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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