Pimelic acid, 2-methylpropyl pentadecyl ester

Inchi: InChI=1S/C26H50O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-19-22-29-25(27)20-17-16-18-21
InchiKey: BGOWVNMICCCTOQ-UHFFFAOYSA-N
Formula: C26H50O4
SMILES: CCCCCCCCCCCCCCCOC(=O)CCCCCC(=O)OCC(C)C
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
mcvol	392.080	ml/mol	McGowan Method
pc	765.64	kPa	Joback Method
rinpol	2929.00		NIST Webbook
rinpol	2929.00		NIST Webbook
tb	946.42	K	Joback Method
tc	1164.49	K	Joback Method
tf	512.10	K	Joback Method
vc	1.534	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1345.59	J/mol×K	946.42	Joback Method
cpg	1366.80	J/mol×K	982.76	Joback Method
cpg	1386.34	J/mol×K	1019.11	Joback Method
cpg	1404.25	J/mol×K	1055.45	Joback Method
cpg	1420.58	J/mol×K	1091.80	Joback Method
cpg	1435.40	J/mol×K	1128.14	Joback Method
cpg	1448.73	J/mol×K	1164.49	Joback Method
dvisc	0.0004671	Pa×s	512.10	Joback Method

dvisc	0.0001988	Pa×s	584.49	Joback Method
dvisc	0.0001021	Pa×s	656.87	Joback Method
dvisc	0.0000599	Pa×s	729.26	Joback Method
dvisc	0.0000387	Pa×s	801.65	Joback Method
dvisc	0.0000268	Pa×s	874.03	Joback Method
dvisc	0.0000197	Pa×s	946.42	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U393861&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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