Pimelic acid, dodecyl 2-methylbutyl ester

Inchi: InChI=1S/C24H46O4/c1-4-6-7-8-9-10-11-12-13-17-20-27-23(25)18-15-14-16-19-24(26)2
InchiKey: RPOJOPPESYNXPE-UHFFFAOYSA-N
Formula: C24H46O4
SMILES: CCCCCCCCCCCCOC(=O)CCCCCC(=O)OCC(C)CC
Mol. weight [g/mol]: 398.62

Physical Properties

Property code	Value	Unit	Source
gf	-319.08	kJ/mol	Joback Method
hf	-1033.57	kJ/mol	Joback Method
hfus	59.97	kJ/mol	Joback Method
hvap	86.94	kJ/mol	Joback Method
log10ws	-7.35		Crippen Method
logp	6.990		Crippen Method
mcvol	363.900	ml/mol	McGowan Method
pc	853.96	kPa	Joback Method
rinpol	2711.00		NIST Webbook
rinpol	2711.00		NIST Webbook
tb	900.66	K	Joback Method
tc	1103.57	K	Joback Method
tf	489.56	K	Joback Method
vc	1.421	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1218.00	J/mol×K	900.66	Joback Method
cpg	1238.11	J/mol×K	934.48	Joback Method
cpg	1256.81	J/mol×K	968.30	Joback Method
cpg	1274.13	J/mol×K	1002.12	Joback Method
cpg	1290.12	J/mol×K	1035.94	Joback Method
cpg	1304.80	J/mol×K	1069.75	Joback Method
cpg	1318.20	J/mol×K	1103.57	Joback Method
dvisc	0.0006076	Pa×s	489.56	Joback Method

dvisc	0.0002626	Pa×s	558.08	Joback Method
dvisc	0.0001364	Pa×s	626.59	Joback Method
dvisc	0.0000806	Pa×s	695.11	Joback Method
dvisc	0.0000523	Pa×s	763.63	Joback Method
dvisc	0.0000365	Pa×s	832.14	Joback Method
dvisc	0.0000269	Pa×s	900.66	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=U406655&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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