

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)CCCCC(=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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0002626	Paxs	558.08	Joback Method
dvisc	0.0001364	Paxs	626.59	Joback Method
dvisc	0.0000806	Paxs	695.11	Joback Method
dvisc	0.0000523	Paxs	763.63	Joback Method
dvisc	0.0000365	Paxs	832.14	Joback Method
dvisc	0.0000269	Paxs	900.66	Joback Method

Sources

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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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