

Pimelic acid, dodecyl 3-methyl-2-pentyl ester

Inchi:	InChI=1S/C25H48O4/c1-5-7-8-9-10-11-12-13-14-18-21-28-24(26)19-16-15-17-20-25(27)
InchiKey:	FRSYABLGHJAURB-UHFFFAOYSA-N
Formula:	C25H48O4
SMILES:	CCCCCCCCCCCCOC(=O)CCCCC(=O)OC(C)C(C)CC
Mol. weight [g/mol]:	412.65

Physical Properties

Property code	Value	Unit	Source
gf	-313.10	kJ/mol	Joback Method
hf	-1059.49	kJ/mol	Joback Method
hfus	59.03	kJ/mol	Joback Method
hvap	88.78	kJ/mol	Joback Method
log10ws	-7.88		Crippen Method
logp	7.379		Crippen Method
mvol	377.990	ml/mol	McGowan Method
pc	811.68	kPa	Joback Method
rinpol	2756.00		NIST Webbook
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tb	923.10	K	Joback Method
tc	1132.09	K	Joback Method
tf	485.83	K	Joback Method
vc	1.472	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1281.95	J/molxK	923.10	Joback Method
cpg	1302.47	J/molxK	957.93	Joback Method
cpg	1321.46	J/molxK	992.76	Joback Method
cpg	1338.96	J/molxK	1027.60	Joback Method
cpg	1355.01	J/molxK	1062.43	Joback Method
cpg	1369.65	J/molxK	1097.26	Joback Method
cpg	1382.92	J/molxK	1132.09	Joback Method
dvisc	0.0006234	Paxs	485.83	Joback Method

dvisc	0.0002451	Paxs	558.71	Joback Method
dvisc	0.0001196	Paxs	631.59	Joback Method
dvisc	0.0000676	Paxs	704.47	Joback Method
dvisc	0.0000426	Paxs	777.34	Joback Method
dvisc	0.0000290	Paxs	850.22	Joback Method
dvisc	0.0000210	Paxs	923.10	Joback Method

Sources

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=U406602&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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