

Pimelic acid, heptyl undecyl ester

Inchi:	InChI=1S/C25H48O4/c1-3-5-7-9-10-11-12-14-19-23-29-25(27)21-17-15-16-20-24(26)28-
InchiKey:	LMMGIYGIDYDPMA-UHFFFAOYSA-N
Formula:	C25H48O4
SMILES:	CCCCCCCCCOC(=O)CCCCC(=O)OCCCCCCC
Mol. weight [g/mol]:	412.65

Physical Properties

Property code	Value	Unit	Source
gf	-308.22	kJ/mol	Joback Method
hf	-1048.93	kJ/mol	Joback Method
hfus	66.08	kJ/mol	Joback Method
hvap	89.56	kJ/mol	Joback Method
log10ws	-8.01		Crippen Method
logp	7.524		Crippen Method
mvol	377.990	ml/mol	McGowan Method
pc	804.33	kPa	Joback Method
rinpol	2029.00		NIST Webbook
rinpol	2029.00		NIST Webbook
tb	923.98	K	Joback Method
tc	1135.00	K	Joback Method
tf	515.83	K	Joback Method
vc	1.484	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1281.17	J/molxK	923.98	Joback Method
cpg	1301.94	J/molxK	959.15	Joback Method
cpg	1321.17	J/molxK	994.32	Joback Method
cpg	1338.92	J/molxK	1029.49	Joback Method
cpg	1355.21	J/molxK	1064.66	Joback Method
cpg	1370.09	J/molxK	1099.83	Joback Method
cpg	1383.60	J/molxK	1135.00	Joback Method
dvisc	0.0004642	Paxs	515.83	Joback Method

dvisc	0.0002153	Paxs	583.86	Joback Method
dvisc	0.0001173	Paxs	651.88	Joback Method
dvisc	0.0000716	Paxs	719.90	Joback Method
dvisc	0.0000476	Paxs	787.93	Joback Method
dvisc	0.0000338	Paxs	855.95	Joback Method
dvisc	0.0000252	Paxs	923.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406517&Units=SI
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

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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