

Pimelic acid, 2,4,4-trimethylpentyl undecyl ester

Inchi:	InChI=1S/C26H50O4/c1-6-7-8-9-10-11-12-13-17-20-29-24(27)18-15-14-16-19-25(28)30-
InchiKey:	MAJKMBMSIXNRLO-UHFFFAOYSA-N
Formula:	C26H50O4
SMILES:	CCCCCCCCCOC(=O)CCCCC(=O)OCC(C)CC(C)(C)C
Mol. weight [g/mol]:	426.67

Physical Properties

Property code	Value	Unit	Source
gf	-299.40	kJ/mol	Joback Method
hf	-1083.60	kJ/mol	Joback Method
hfus	57.73	kJ/mol	Joback Method
hvap	90.10	kJ/mol	Joback Method
log10ws	-7.95		Crippen Method
logp	7.626		Crippen Method
mcvol	392.080	ml/mol	McGowan Method
pc	773.75	kPa	Joback Method
rinpol	2001.00		NIST Webbook
rinpol	2001.00		NIST Webbook
tb	943.19	K	Joback Method
tc	1157.23	K	Joback Method
tf	514.52	K	Joback Method
vc	1.522	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1345.34	J/molxK	943.19	Joback Method
cpg	1366.13	J/molxK	978.86	Joback Method
cpg	1385.41	J/molxK	1014.54	Joback Method
cpg	1403.24	J/molxK	1050.21	Joback Method
cpg	1419.69	J/molxK	1085.88	Joback Method
cpg	1434.82	J/molxK	1121.56	Joback Method
cpg	1448.69	J/molxK	1157.23	Joback Method
dvisc	0.0004231	Paxs	514.52	Joback Method

dvisc	0.0001730	Paxs	585.97	Joback Method
dvisc	0.0000859	Paxs	657.41	Joback Method
dvisc	0.0000490	Paxs	728.86	Joback Method
dvisc	0.0000308	Paxs	800.30	Joback Method
dvisc	0.0000210	Paxs	871.75	Joback Method
dvisc	0.0000151	Paxs	943.19	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=U406479&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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