

Pimelic acid, 3-chlorophenyl tridecyl ester

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C26H41ClO4/c1-2-3-4-5-6-7-8-9-10-11-15-21-30-25(28)19-13-12-14-20-26(29)

CWOKGCNFAHSSLY-UHFFFAOYSA-N

C26H41ClO4

CCCCCCCCCCCCCOC(=O)CCCCC(=O)Oc1cccc(Cl)c1

453.05

Physical Properties

Property code	Value	Unit	Source
gf	-208.95	kJ/mol	Joback Method
hf	-860.25	kJ/mol	Joback Method
hfus	66.52	kJ/mol	Joback Method
hvap	99.10	kJ/mol	Joback Method
log10ws	-8.87		Crippen Method
logp	8.050		Crippen Method
mcvol	380.560	ml/mol	McGowan Method
pc	894.80	kPa	Joback Method
rinpol	2904.00		NIST Webbook
rinpol	2904.00		NIST Webbook
tb	1015.95	K	Joback Method
tc	1245.61	K	Joback Method
tf	595.96	K	Joback Method
vc	1.480	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1269.77	J/molxK	1015.95	Joback Method
cpg	1286.19	J/molxK	1054.23	Joback Method
cpg	1301.01	J/molxK	1092.50	Joback Method
cpg	1314.29	J/molxK	1130.78	Joback Method
cpg	1326.09	J/molxK	1169.06	Joback Method
cpg	1336.48	J/molxK	1207.34	Joback Method
cpg	1345.50	J/molxK	1245.61	Joback Method
dvisc	0.0002398	Paxs	595.96	Joback Method

dvisc	0.0001260	Paxs	665.96	Joback Method
dvisc	0.0000748	Paxs	735.96	Joback Method
dvisc	0.0000486	Paxs	805.95	Joback Method
dvisc	0.0000339	Paxs	875.95	Joback Method
dvisc	0.0000249	Paxs	945.95	Joback Method
dvisc	0.0000191	Paxs	1015.95	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=U416678&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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