

Pimelic acid, 3,5-dichlorobenzyl heptyl ester

Inchi:	InChI=1S/C21H30Cl2O4/c1-2-3-4-5-9-12-26-20(24)10-7-6-8-11-21(25)27-16-17-13-18(2)
InchiKey:	DUEUSKPYAOZMOY-UHFFFAOYSA-N
Formula:	C21H30Cl2O4
SMILES:	CCCCCCCOC(=O)CCCCC(=O)OCc1cc(Cl)cc(Cl)c1
Mol. weight [g/mol]:	417.37

Physical Properties

Property code	Value	Unit	Source
gf	-272.61	kJ/mol	Joback Method
hf	-784.26	kJ/mol	Joback Method
hfus	57.38	kJ/mol	Joback Method
hvap	93.02	kJ/mol	Joback Method
log10ws	-7.31		Crippen Method
logp	6.501		Crippen Method
mcvol	322.350	ml/mol	McGowan Method
pc	1176.85	kPa	Joback Method
rinpol	2896.00		NIST Webbook
rinpol	2896.00		NIST Webbook
tb	943.96	K	Joback Method
tc	1158.36	K	Joback Method
tf	582.05	K	Joback Method
vc	1.250	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	988.45	J/molxK	943.96	Joback Method
cpg	1045.81	J/molxK	1122.62	Joback Method
cpg	1036.72	J/molxK	1086.89	Joback Method
cpg	1026.47	J/molxK	1051.16	Joback Method
cpg	1015.03	J/molxK	1015.43	Joback Method
cpg	1002.36	J/molxK	979.69	Joback Method
cpg	1053.76	J/molxK	1158.36	Joback Method
dvisc	0.0000353	Paxs	943.96	Joback Method

dvisc	0.0000448	Paxs	883.64	Joback Method
dvisc	0.0000589	Paxs	823.32	Joback Method
dvisc	0.0000809	Paxs	763.00	Joback Method
dvisc	0.0001172	Paxs	702.69	Joback Method
dvisc	0.0001821	Paxs	642.37	Joback Method
dvisc	0.0003100	Paxs	582.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406688&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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