

Pimelic acid, decyl 3,4-dichlorophenyl ester

Inchi:	InChI=1S/C23H34Cl2O4/c1-2-3-4-5-6-7-8-12-17-28-22(26)13-10-9-11-14-23(27)29-19-15
InchiKey:	BTDKRZPYLWWDOX-UHFFFAOYSA-N
Formula:	C23H34Cl2O4
SMILES:	CCCCCCCCCOC(=O)CCCCC(=O)Oc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]:	445.42

Physical Properties

Property code	Value	Unit	Source
gf	-255.77	kJ/mol	Joback Method
hf	-825.54	kJ/mol	Joback Method
hfus	62.56	kJ/mol	Joback Method
hvap	97.47	kJ/mol	Joback Method
log10ws	-8.30		Crippen Method
logp	7.533		Crippen Method
mvol	350.530	ml/mol	McGowan Method
pc	1035.90	kPa	Joback Method
rinpol	3083.00		NIST Webbook
rinpol	3083.00		NIST Webbook
tb	989.72	K	Joback Method
tc	1211.74	K	Joback Method
tf	604.59	K	Joback Method
vc	1.361	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1108.77	J/molxK	989.72	Joback Method
cpg	1166.86	J/molxK	1174.74	Joback Method
cpg	1157.88	J/molxK	1137.74	Joback Method
cpg	1147.62	J/molxK	1100.73	Joback Method
cpg	1136.04	J/molxK	1063.73	Joback Method
cpg	1123.10	J/molxK	1026.72	Joback Method
cpg	1174.60	J/molxK	1211.74	Joback Method
dvisc	0.0000260	Paxs	989.72	Joback Method

dvisc	0.0000333	Paxs	925.53	Joback Method
dvisc	0.0000440	Paxs	861.34	Joback Method
dvisc	0.0000610	Paxs	797.15	Joback Method
dvisc	0.0000895	Paxs	732.97	Joback Method
dvisc	0.0001412	Paxs	668.78	Joback Method
dvisc	0.0002456	Paxs	604.59	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=U416737&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	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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