

Pimelic acid, 3,5-dichlorobenzyl hexyl ester

Inchi:	InChI=1S/C20H28Cl2O4/c1-2-3-4-8-11-25-19(23)9-6-5-7-10-20(24)26-15-16-12-17(21)14
InchiKey:	VDFQTYWCLLGGWPT-UHFFFAOYSA-N
Formula:	C20H28Cl2O4
SMILES:	CCCCCOC(=O)CCCCC(=O)OCc1cc(Cl)cc(Cl)c1
Mol. weight [g/mol]:	403.34

Physical Properties

Property code	Value	Unit	Source
gf	-281.03	kJ/mol	Joback Method
hf	-763.62	kJ/mol	Joback Method
hfus	54.79	kJ/mol	Joback Method
hvap	90.80	kJ/mol	Joback Method
log10ws	-6.89		Crippen Method
logp	6.111		Crippen Method
mvol	308.260	ml/mol	McGowan Method
pc	1258.37	kPa	Joback Method
rinpol	2796.00		NIST Webbook
rinpol	2796.00		NIST Webbook
tb	921.08	K	Joback Method
tc	1133.06	K	Joback Method
tf	570.78	K	Joback Method
vc	1.194	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	929.13	J/molxK	921.08	Joback Method
cpg	942.84	J/molxK	956.41	Joback Method
cpg	955.36	J/molxK	991.74	Joback Method
cpg	966.72	J/molxK	1027.07	Joback Method
cpg	976.94	J/molxK	1062.40	Joback Method
cpg	986.04	J/molxK	1097.73	Joback Method
cpg	994.05	J/molxK	1133.06	Joback Method
dvisc	0.0003466	Paxs	570.78	Joback Method

dvisc	0.0002059	Paxs	629.16	Joback Method
dvisc	0.0001336	Paxs	687.55	Joback Method
dvisc	0.0000928	Paxs	745.93	Joback Method
dvisc	0.0000679	Paxs	804.31	Joback Method
dvisc	0.0000519	Paxs	862.70	Joback Method
dvisc	0.0000410	Paxs	921.08	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=U406687&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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