

Pimelic acid, butyl 3,4-dichlorophenyl ester

Inchi:	InChI=1S/C17H22Cl2O4/c1-2-3-11-22-16(20)7-5-4-6-8-17(21)23-13-9-10-14(18)15(19)12
InchiKey:	NLXKCBLVUZBFAJ-UHFFFAOYSA-N
Formula:	C17H22Cl2O4
SMILES:	CCCCOC(=O)CCCCC(=O)Oc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]:	361.26

Physical Properties

Property code	Value	Unit	Source
gf	-306.29	kJ/mol	Joback Method
hf	-701.70	kJ/mol	Joback Method
hfus	47.02	kJ/mol	Joback Method
hvap	84.12	kJ/mol	Joback Method
log10ws	-5.79		Crippen Method
logp	5.193		Crippen Method
mvol	265.990	ml/mol	McGowan Method
pc	1561.05	kPa	Joback Method
rinpol	2473.00		NIST Webbook
rinpol	2473.00		NIST Webbook
tb	852.44	K	Joback Method
tc	1062.07	K	Joback Method
tf	536.97	K	Joback Method
vc	1.026	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	755.26	J/mol×K	852.44	Joback Method
cpg	768.31	J/mol×K	887.38	Joback Method
cpg	780.32	J/mol×K	922.32	Joback Method
cpg	791.29	J/mol×K	957.25	Joback Method
cpg	801.26	J/mol×K	992.19	Joback Method
cpg	810.22	J/mol×K	1027.13	Joback Method
cpg	818.20	J/mol×K	1062.07	Joback Method
dvisc	0.0004746	Paxs	536.97	Joback Method

dvisc	0.0002921	Paxs	589.55	Joback Method
dvisc	0.0001947	Paxs	642.13	Joback Method
dvisc	0.0001380	Paxs	694.70	Joback Method
dvisc	0.0001026	Paxs	747.28	Joback Method
dvisc	0.0000794	Paxs	799.86	Joback Method
dvisc	0.0000634	Paxs	852.44	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=U416730&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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