

Pimelic acid, 3,5-dichlorobenzyl isobutyl ester

Inchi: InChI=1S/C18H24Cl2O4/c1-13(2)11-23-17(21)6-4-3-5-7-18(22)24-12-14-8-15(19)10-16(20)
InchiKey: MNJPDUWPZVYKOO-UHFFFAOYSA-N
Formula: C18H24Cl2O4
SMILES: CC(C)COC(=O)CCCCC(=O)OCc1cc(Cl)cc(Cl)c1
Mol. weight [g/mol]: 375.29

Physical Properties

Property code	Value	Unit	Source
gf	-300.31	kJ/mol	Joback Method
hf	-727.62	kJ/mol	Joback Method
hfus	46.08	kJ/mol	Joback Method
hvap	85.96	kJ/mol	Joback Method
log10ws	-5.81		Crippen Method
logp	5.186		Crippen Method
mcvol	280.080	ml/mol	McGowan Method
pc	1457.90	kPa	Joback Method
rinpol	2548.00		NIST Webbook
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tb	874.88	K	Joback Method
tc	1086.47	K	Joback Method
tf	533.24	K	Joback Method
vc	1.075	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	813.01	J/molxK	874.88	Joback Method
cpg	826.39	J/molxK	910.15	Joback Method
cpg	838.66	J/molxK	945.41	Joback Method
cpg	849.82	J/molxK	980.68	Joback Method
cpg	859.90	J/molxK	1015.94	Joback Method
cpg	868.92	J/molxK	1051.21	Joback Method
cpg	876.88	J/molxK	1086.47	Joback Method
dvisc	0.0004701	Paxs	533.24	Joback Method

dvisc	0.0002706	Paxs	590.18	Joback Method
dvisc	0.0001716	Paxs	647.12	Joback Method
dvisc	0.0001172	Paxs	704.06	Joback Method
dvisc	0.0000847	Paxs	761.00	Joback Method
dvisc	0.0000641	Paxs	817.94	Joback Method
dvisc	0.0000503	Paxs	874.88	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=U406683&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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