

Benzoic acid, (2,6-dichlorophenyl)metyl ester

Inchi:	InChI=1S/C14H10Cl2O2/c15-12-7-4-8-13(16)11(12)9-18-14(17)10-5-2-1-3-6-10/h1-8H,9
InchiKey:	DOGFLSFWCPMNOH-UHFFFAOYSA-N
Formula:	C14H10Cl2O2
SMILES:	O=C(OCc1c(Cl)cccc1Cl)c1ccccc1
Mol. weight [g/mol]:	281.13

Physical Properties

Property code	Value	Unit	Source
gf	14.78	kJ/mol	Joback Method
hf	-158.45	kJ/mol	Joback Method
hfus	30.50	kJ/mol	Joback Method
hvap	70.56	kJ/mol	Joback Method
log10ws	-5.19		Crippen Method
logp	4.350		Crippen Method
mvol	192.520	ml/mol	McGowan Method
pc	2608.40	kPa	Joback Method
rinpol	2176.00		NIST Webbook
rinpol	2176.00		NIST Webbook
tb	734.19	K	Joback Method
tc	983.40	K	Joback Method
tf	457.42	K	Joback Method
vc	0.726	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	461.35	J/molxK	734.19	Joback Method
cpg	512.54	J/molxK	941.87	Joback Method
cpg	504.32	J/molxK	900.33	Joback Method
cpg	495.13	J/molxK	858.80	Joback Method
cpg	484.94	J/molxK	817.26	Joback Method
cpg	473.70	J/molxK	775.73	Joback Method
cpg	519.85	J/molxK	983.40	Joback Method
dvisc	0.0001289	Paxs	734.19	Joback Method

dvisc	0.0001591	Paxs	688.06	Joback Method
dvisc	0.0002024	Paxs	641.93	Joback Method
dvisc	0.0002673	Paxs	595.81	Joback Method
dvisc	0.0003697	Paxs	549.68	Joback Method
dvisc	0.0005428	Paxs	503.55	Joback Method
dvisc	0.0008610	Paxs	457.42	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368899&Units=SI

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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