Benzoic acid, (2,5-dichlorophenyl)methyl ester

Inchi: InChI=1S/C14H10Cl2O2/c15-12-6-7-13(16)11(8-12)9-18-14(17)10-4-2-1-3-5-10/h1-8H,9
InchiKey: HLVHDLIRQRTRSQ-UHFFFAOYSA-N
Formula: C14H10Cl2O2
SMILES: O=C(OCc1cc(Cl)ccc1Cl)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
mcvol	192.520	ml/mol	McGowan Method
pc	2608.40	kPa	Joback Method
rinpol	2174.00		NIST Webbook
rinpol	2174.00		NIST Webbook
tb	734.19	K	Joback Method
tc	983.40	K	Joback Method
tf	457.42	K	Joback Method
vc	0.726	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0001591	Pa×s	688.06	Joback Method
dvisc	0.0002024	Pa×s	641.93	Joback Method
dvisc	0.0002673	Pa×s	595.81	Joback Method
dvisc	0.0003697	Pa×s	549.68	Joback Method
dvisc	0.0005428	Pa×s	503.55	Joback Method
dvisc	0.0008610	Pa×s	457.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368895&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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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