Benzoic acid, 3,4-dichlorophenyl ester

Inchi: InChI=1S/C13H8Cl2O2/c14-11-7-6-10(8-12(11)15)17-13(16)9-4-2-1-3-5-9/h1-8H
InchiKey: RPLHUYYGJWQIFA-UHFFFAOYSA-N
Formula: C13H8Cl2O2
SMILES: O=C(Oc1ccc(Cl)c(Cl)c1)c1ccccc1
Mol. weight [g/mol]: 267.11

Physical Properties

Property code	Value	Unit	Source
gf	6.36	kJ/mol	Joback Method
hf	-137.81	kJ/mol	Joback Method
hfus	27.91	kJ/mol	Joback Method
hvap	68.33	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	4.213		Crippen Method
mcvol	178.430	ml/mol	McGowan Method
pc	2884.30	kPa	Joback Method
rinpol	2103.00		NIST Webbook
rinpol	2103.00		NIST Webbook
tb	711.31	K	Joback Method
tc	966.18	K	Joback Method
tf	446.15	K	Joback Method
vc	0.669	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	410.63	J/mol×K	711.31	Joback Method
cpg	422.43	J/mol×K	753.79	Joback Method
cpg	433.14	J/mol×K	796.27	Joback Method
cpg	442.82	J/mol×K	838.75	Joback Method
cpg	451.51	J/mol×K	881.22	Joback Method
cpg	459.25	J/mol×K	923.70	Joback Method
cpg	466.10	J/mol×K	966.18	Joback Method
dvisc	0.0009179	Pa×s	446.15	Joback Method

dvisc	0.0005874	Pa×s	490.34	Joback Method
dvisc	0.0004047	Pa×s	534.54	Joback Method
dvisc	0.0002951	Pa×s	578.73	Joback Method
dvisc	0.0002251	Pa×s	622.92	Joback Method
dvisc	0.0001780	Pa×s	667.12	Joback Method
dvisc	0.0001449	Pa×s	711.31	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357802&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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