Dichloroacetamide, N-(2-fluorophenyl)-

Inchi: InChI=1S/C8H6Cl2FNO/c9-7(10)8(13)12-6-4-2-1-3-5(6)11/h1-4,7H,(H,12,13)
InchiKey: QTWULMASGKOCHL-UHFFFAOYSA-N
Formula: C8H6Cl2FNO
SMILES: O=C(Nc1ccccc1F)C(Cl)Cl
Mol. weight [g/mol]: 222.04

Physical Properties

Property code	Value	Unit	Source
gf	-141.38	kJ/mol	Joback Method
hf	-275.37	kJ/mol	Joback Method
hfus	24.78	kJ/mol	Joback Method
hvap	57.09	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	2.568		Crippen Method
mcvol	137.620	ml/mol	McGowan Method
pc	3439.94	kPa	Joback Method
rinpol	1415.00		NIST Webbook
tb	591.83	K	Joback Method
tc	817.76	K	Joback Method
tf	366.88	K	Joback Method
vc	0.526	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	288.99	J/mol×K	591.83	Joback Method
cpg	298.70	J/mol×K	629.49	Joback Method
cpg	307.69	J/mol×K	667.14	Joback Method
cpg	315.97	J/mol×K	704.80	Joback Method
cpg	323.58	J/mol×K	742.45	Joback Method
cpg	330.56	J/mol×K	780.11	Joback Method
cpg	336.95	J/mol×K	817.76	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308631&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

Legend

cpg:	Ideal gas heat capacity
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