N,N-Diethyl(2-chloro-1,1,2-trifluoroethyl)amine

Inchi: InChI=1S/C6H11ClF3N/c1-3-11(4-2)6(9,10)5(7)8/h5H,3-4H2,1-2H3
InchiKey: BDZHKUAKSMWSAJ-UHFFFAOYSA-N
Formula: C6H11ClF3N
SMILES: CCN(CC)C(F)(F)C(F)Cl
Mol. weight [g/mol]: 189.61
CAS: 357-83-5

Physical Properties

Property code	Value	Unit	Source
gf	-485.54	kJ/mol	Joback Method
hf	-717.74	kJ/mol	Joback Method
hfus	16.82	kJ/mol	Joback Method
hvap	31.24	kJ/mol	Joback Method
log10ws	-2.33		Crippen Method
logp	2.455		Crippen Method
mcvol	122.930	ml/mol	McGowan Method
pc	2654.29	kPa	Joback Method
tb	380.69	K	Joback Method
tc	539.13	K	Joback Method
tf	208.96	K	Joback Method
vc	0.475	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.70	J/mol×K	380.69	Joback Method
cpg	250.39	J/mol×K	407.10	Joback Method
cpg	261.49	J/mol×K	433.50	Joback Method
cpg	272.02	J/mol×K	459.91	Joback Method
cpg	282.01	J/mol×K	486.32	Joback Method
cpg	291.47	J/mol×K	512.72	Joback Method
cpg	300.43	J/mol×K	539.13	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	311.00	K	1.30	NIST Webbook

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=C357835&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume