1-Chloro-1,1-dibromotrifluoroethane

Other names: 1-Chloro-1,1-dibromotrifluoroethane
1,1-Dibromo-1-chlorotrifluoroethane
Inchi: InChI=1S/C2Br2ClF3/c3-1(4,5)2(6,7)8
InchiKey: WGIRTDAEWOUFQR-UHFFFAOYSA-N
Formula: C2Br2ClF3
SMILES: FC(F)(F)C(Cl)(Br)Br
Mol. weight [g/mol]: 276.28

Physical Properties

Property code	Value	Unit	Source
af	0.3251		Cheméo Relay (1.0)
gf	-596.08	kJ/mol	Joback Method
hf	-625.72	kJ/mol	Cheméo Relay (1.0)
hfus	10.12	kJ/mol	Joback Method
hvap	30.16	kJ/mol	Cheméo Relay (1.0)
ie	11.19	eV	Cheméo Relay (1.0)
log10ws	-3.01		Cheméo Relay (1.0)
logp	3.231		Crippen Method
mcvol	91.590	ml/mol	McGowan Method
pc	5058.59	kPa	Joback Method
tb	364.50 ± 0.50	K	NIST Webbook
tc	522.66	K	Cheméo Relay (1.0)
tf	246.75	K	Cheméo Relay (1.0)
vc	0.337	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	139.80	J/mol×K	406.26	Joback Method
cpg	145.28	J/mol×K	441.48	Joback Method
cpg	149.99	J/mol×K	476.69	Joback Method
cpg	154.00	J/mol×K	511.91	Joback Method
cpg	157.38	J/mol×K	547.13	Joback Method
cpg	160.18	J/mol×K	582.35	Joback Method

cpg	162.48	J/mol×K	617.56	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C754176&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume