Propane, 3-bromo-1-chloro-1,1-difluoro-

Inchi: InChI=1S/C3H4BrClF2/c4-2-1-3(5,6)7/h1-2H2
InchiKey: KWDSTKTWEBLQIW-UHFFFAOYSA-N
Formula: C3H4BrClF2
SMILES: FC(F)(Cl)CCBr
Mol. weight [g/mol]: 193.42
CAS: 460-29-7

Physical Properties

Property code	Value	Unit	Source
gf	-410.01	kJ/mol	Joback Method
hf	-495.63	kJ/mol	Joback Method
hfus	11.75	kJ/mol	Joback Method
hvap	30.16	kJ/mol	Joback Method
log10ws	-2.47		Crippen Method
logp	2.603		Crippen Method
mcvol	86.410	ml/mol	McGowan Method
pc	4189.32	kPa	Joback Method
tb	366.94	K	Joback Method
tc	553.34	K	Joback Method
tf	216.89	K	Joback Method
vc	0.340	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	135.02	J/mol×K	366.94	Joback Method
cpg	141.74	J/mol×K	398.01	Joback Method
cpg	147.95	J/mol×K	429.07	Joback Method
cpg	153.70	J/mol×K	460.14	Joback Method
cpg	159.01	J/mol×K	491.20	Joback Method
cpg	163.91	J/mol×K	522.27	Joback Method
cpg	168.42	J/mol×K	553.34	Joback Method

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=C460297&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume