Dibromofluoroacetic acid

Inchi: InChI=1S/C2HBr2FO2/c3-2(4,5)1(6)7/h(H,6,7)
InchiKey: NWIYDZBYJAJLNC-UHFFFAOYSA-N
Formula: C2HBr2FO2
SMILES: O=C(O)C(F)(Br)Br
Mol. weight [g/mol]: 235.84
CAS: 353-99-1

Physical Properties

Property code	Value	Unit	Source
gf	-463.11	kJ/mol	Joback Method
hf	-501.62	kJ/mol	Joback Method
hfus	12.86	kJ/mol	Joback Method
hvap	54.23	kJ/mol	Joback Method
log10ws	-1.58		Crippen Method
logp	1.484		Crippen Method
mcvol	83.250	ml/mol	McGowan Method
pc	7654.34	kPa	Joback Method
tb	519.57	K	Joback Method
tc	731.24	K	Joback Method
tf	345.66	K	Joback Method
vc	0.303	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	133.57	J/mol×K	519.57	Joback Method
cpg	136.82	J/mol×K	554.85	Joback Method
cpg	139.66	J/mol×K	590.13	Joback Method
cpg	142.13	J/mol×K	625.41	Joback Method
cpg	144.29	J/mol×K	660.69	Joback Method
cpg	146.17	J/mol×K	695.96	Joback Method
cpg	147.80	J/mol×K	731.24	Joback Method
hvapt	60.20	kJ/mol	435.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	403.00	K	8.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.66336e+01
Coeff. B	-4.67402e+03
Coeff. C	-8.19900e+01
Temperature range (K), min.	367.93
Temperature range (K), max.	494.81

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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=C353991&Units=SI

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume