1,2-Dibromo-1,1,2-trifluoroethane

Other names: Ethane, 1,2-dibromo-1,1,2-trifluoro-
Inchi: InChI=1S/C2HBr2F3/c3-1(5)2(4,6)7/h1H
InchiKey: UREJNEBJDURREH-UHFFFAOYSA-N
Formula: C2HBr2F3
SMILES: FC(Br)C(F)(F)Br
Mol. weight [g/mol]: 241.83
CAS: 354-04-1

Physical Properties

Property code	Value	Unit	Source
gf	-589.43	kJ/mol	Joback Method
hf	-634.31	kJ/mol	Joback Method
hfus	9.81	kJ/mol	Joback Method
hvap	28.78	kJ/mol	Joback Method
log10ws	-2.79		Crippen Method
logp	2.665		Crippen Method
mcvol	79.350	ml/mol	McGowan Method
pc	5251.00	kPa	Joback Method
tb	349.00 ± 2.00	K	NIST Webbook
tb	349.00 ± 2.00	K	NIST Webbook
tb	349.00	K	NIST Webbook
tc	565.45	K	Joback Method
tf	221.09	K	Joback Method
vc	0.308	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	118.33	J/mol×K	371.62	Joback Method
cpg	123.60	J/mol×K	403.93	Joback Method
cpg	128.35	J/mol×K	436.23	Joback Method
cpg	132.62	J/mol×K	468.54	Joback Method
cpg	136.44	J/mol×K	500.84	Joback Method
cpg	139.85	J/mol×K	533.15	Joback Method

cpg	142.88	J/mol×K	565.45	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56591e+01
Coeff. B	-3.85322e+03
Temperature range (K), min.	250.67
Temperature range (K), max.	372.58

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C354041&Units=SI
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

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf:	Normal melting (fusion) point
vc:	Critical Volume

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