

Ethane, 1,2-dibromo-1,1,2-trifluoro-

Other names:	1,2-dibromo-1,1,2-trifluoroethane
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
hf	-624.88	kJ/mol	Cheméo Relay (1.0)
hfus	9.81	kJ/mol	Joback Method
hvap	34.39	kJ/mol	Cheméo Relay (1.0)
ie	11.04	eV	Cheméo Relay (1.0)
logp	2.665		Crippen Method
mcvol	79.350	ml/mol	McGowan Method
pc	5251.00	kPa	Joback Method
tb	349.00	K	NIST Webbook
tb	349.00 ± 2.00	K	NIST Webbook
tb	349.00 ± 2.00	K	NIST Webbook
tc	528.44	K	Cheméo Relay (1.0)
tf	150.56	K	Cheméo Relay (1.0)
vc	0.313	m3/kmol	Cheméo Relay (1.0)

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	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.56591e+01
Coeff. B	-3.85322e+03
Temperature range (K), min.	250.67
Temperature range (K), max.	372.58

Sources

The Yaws Handbook of Vapor
Pressure:
NIST Webbook:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>
<http://webbook.nist.gov/cgi/cbook.cgi?ID=C354041&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

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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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