Butane, 2,2-difluoro

Other names: 2,2-Difluorobutane
Inchi: InChI=1S/C4H8F2/c1-3-4(2,5)6/h3H2,1-2H3
InchiKey: IIADOUMJKYSCPM-UHFFFAOYSA-N
Formula: C4H8F2
SMILES: CCC(C)(F)F
Mol. weight [g/mol]: 94.10
CAS: 353-81-1

Physical Properties

Property code	Value	Unit	Source
gf	-403.98	kJ/mol	Joback Method
hf	-526.86	kJ/mol	Joback Method
hfus	4.86	kJ/mol	Joback Method
hvap	21.57	kJ/mol	Joback Method
log10ws	-1.81		Crippen Method
logp	2.052		Crippen Method
mcvol	70.760	ml/mol	McGowan Method
pc	3572.80	kPa	Joback Method
rinpol	434.00		NIST Webbook
rinpol	434.00		NIST Webbook
tb	304.00 ± 1.00	K	NIST Webbook
tc	439.30	K	Joback Method
tf	138.44	K	Joback Method
vc	0.284	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	147.86	J/mol×K	413.79	Joback Method
cpg	109.75	J/mol×K	286.23	Joback Method
cpg	118.10	J/mol×K	311.74	Joback Method
cpg	126.07	J/mol×K	337.25	Joback Method
cpg	133.68	J/mol×K	362.76	Joback Method
cpg	140.94	J/mol×K	388.27	Joback Method

cpg	154.46	J/mol×K	439.30	Joback Method
hvapt	30.00	kJ/mol	287.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.32951e+01
Coeff. B	-2.02243e+03
Coeff. C	-7.09140e+01
Temperature range (K), min.	226.40
Temperature range (K), max.	324.24

Sources

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=C353811&Units=SI

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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume