2,3-Butanedithiol

Other names: butane-2,3-dithiol
Inchi: InChI=1S/C4H10S2/c1-3(5)4(2)6/h3-6H,1-2H3
InchiKey: TWWSEEHCVDRRRI-UHFFFAOYSA-N
Formula: C4H10S2
SMILES: CC(S)C(C)S
Mol. weight [g/mol]: 122.25
CAS: 4532-64-3

Physical Properties

Property code	Value	Unit	Source
gf	36.70	kJ/mol	Joback Method
hf	-59.49	kJ/mol	Joback Method
hfus	7.15	kJ/mol	Joback Method
hvap	37.20	kJ/mol	Joback Method
log10ws	-1.86		Crippen Method
logp	1.623		Crippen Method
mcvol	99.920	ml/mol	McGowan Method
pc	4704.19	kPa	Joback Method
tb	415.76	K	Joback Method
tc	645.26	K	Joback Method
tf	177.76	K	Joback Method
vc	0.355	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	173.86	J/mol×K	415.76	Joback Method
cpg	183.94	J/mol×K	454.01	Joback Method
cpg	193.50	J/mol×K	492.26	Joback Method
cpg	202.53	J/mol×K	530.51	Joback Method
cpg	211.07	J/mol×K	568.76	Joback Method
cpg	219.12	J/mol×K	607.01	Joback Method
cpg	226.70	J/mol×K	645.26	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.30164e+01
Coeff. B	-3.39747e+03
Coeff. C	-6.63360e+01
Temperature range (K), min.	333.25
Temperature range (K), max.	507.28

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4532643&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

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