

2-Butene, 1,4-dibromo-

Other names:	1,4-Dibromo-2-butene 1,4-dibromobut-2-ene TL 80
Inchi:	InChI=1S/C4H6Br2/c5-3-1-2-4-6/h1-2H,3-4H2
InchiKey:	RMXLHIUHKIVPAB-UHFFFAOYSA-N
Formula:	C4H6Br2
SMILES:	BrCC=CCBr
Mol. weight [g/mol]:	213.90
CAS:	6974-12-5

Physical Properties

Property code	Value	Unit	Source
gf	91.66	kJ/mol	Joback Method
hf	43.99	kJ/mol	Joback Method
hfus	16.89	kJ/mol	Joback Method
hvap	37.33	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	2.332		Crippen Method
mcvol	97.920	ml/mol	McGowan Method
pc	5015.69	kPa	Joback Method
tb	427.40	K	Joback Method
tc	644.74	K	Joback Method
tf	249.36	K	Joback Method
vc	0.363	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	141.76	J/molxK	427.40	Joback Method
cpg	172.24	J/molxK	608.51	Joback Method
cpg	167.07	J/molxK	572.29	Joback Method
cpg	161.48	J/molxK	536.07	Joback Method
cpg	155.43	J/molxK	499.85	Joback Method
cpg	148.87	J/molxK	463.62	Joback Method

cpg	177.04	J/molxK	644.74	Joback Method
dvisc	0.0003671	Paxs	427.40	Joback Method
dvisc	0.0004552	Paxs	397.73	Joback Method
dvisc	0.0005845	Paxs	368.05	Joback Method
dvisc	0.0007841	Paxs	338.38	Joback Method
dvisc	0.0011129	Paxs	308.71	Joback Method
dvisc	0.0017018	Paxs	279.03	Joback Method
dvisc	0.0028790	Paxs	249.36	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.54127e+01
Coeff. B	-4.00119e+03
Coeff. C	-6.45400e+01
Temperature range (K), min.	329.08
Temperature range (K), max.	472.15

Sources

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=C6974125&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/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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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