2-Ethyl-1,2-dibromobutane

Inchi: InChI=1S/C6H12Br2/c1-3-6(8,4-2)5-7/h3-5H2,1-2H3
InchiKey: UBFOYEMXPUOMHZ-UHFFFAOYSA-N
Formula: C6H12Br2
SMILES: CCC(Br)(CC)CBr
Mol. weight [g/mol]: 243.97

Physical Properties

Property code	Value	Unit	Source
gf	31.12	kJ/mol	Joback Method
hf	-123.26	kJ/mol	Joback Method
hfus	14.45	kJ/mol	Joback Method
hvap	40.52	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	3.335		Crippen Method
mcvol	130.400	ml/mol	McGowan Method
pc	3731.66	kPa	Joback Method
rinpol	1124.00		NIST Webbook
rinpol	1124.00		NIST Webbook
tb	465.77	K	Joback Method
tc	680.86	K	Joback Method
tf	279.40	K	Joback Method
vc	0.484	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	237.14	J/mol×K	465.77	Joback Method
cpg	248.60	J/mol×K	501.62	Joback Method
cpg	259.25	J/mol×K	537.47	Joback Method
cpg	269.14	J/mol×K	573.31	Joback Method
cpg	278.32	J/mol×K	609.16	Joback Method
cpg	286.87	J/mol×K	645.01	Joback Method
cpg	294.82	J/mol×K	680.86	Joback Method
dvisc	0.0041844	Pa×s	279.40	Joback Method

dvisc	0.0022883	Pa×s	310.46	Joback Method
dvisc	0.0013966	Pa×s	341.52	Joback Method
dvisc	0.0009255	Pa×s	372.58	Joback Method
dvisc	0.0006534	Pa×s	403.65	Joback Method
dvisc	0.0004849	Pa×s	434.71	Joback Method
dvisc	0.0003744	Pa×s	465.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R559385&Units=SI
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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume