

Hexane, 2,3-dibromo-, erythro

Inchi:	InChI=1S/C6H12Br2/c1-3-4-6(8)5(2)7/h5-6H,3-4H2,1-2H3/t5-,6+/m1/s1
InchiKey:	CHNCACSQVNDLSU-RITPCOANSA-N
Formula:	C6H12Br2
SMILES:	CCCC(Br)C(C)Br
Mol. weight [g/mol]:	243.97

Physical Properties

Property code	Value	Unit	Source
gf	23.40	kJ/mol	Joback Method
hf	-125.07	kJ/mol	Joback Method
hfus	14.82	kJ/mol	Joback Method
hvap	41.04	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	3.333		Crippen Method
mvol	130.400	ml/mol	McGowan Method
pc	3718.02	kPa	Joback Method
rinpol	1095.00		NIST Webbook
rinpol	1095.00		NIST Webbook
tb	468.12	K	Joback Method
tc	679.14	K	Joback Method
tf	246.98	K	Joback Method
vc	0.483	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.43	J/molxK	468.12	Joback Method
cpg	283.45	J/molxK	643.97	Joback Method
cpg	274.79	J/molxK	608.80	Joback Method
cpg	265.60	J/molxK	573.63	Joback Method
cpg	255.83	J/molxK	538.46	Joback Method
cpg	245.45	J/molxK	503.29	Joback Method
cpg	291.59	J/molxK	679.14	Joback Method
dvisc	0.0003373	Paxs	468.12	Joback Method

dvisc	0.0004452	Paxs	431.26	Joback Method
dvisc	0.0006189	Paxs	394.41	Joback Method
dvisc	0.0009209	Paxs	357.55	Joback Method
dvisc	0.0015014	Paxs	320.69	Joback Method
dvisc	0.0027790	Paxs	283.84	Joback Method
dvisc	0.0061816	Paxs	246.98	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R294598&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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