Hexane, 2,3-dibromo-, threo

Inchi: InChI=1S/C6H12Br2/c1-3-4-6(8)5(2)7/h5-6H,3-4H2,1-2H3/t5-,6-/m0/s1
InchiKey: CHNCACSQVNDLSU-WDSKDSINSA-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
mcvol	130.400	ml/mol	McGowan Method
pc	3718.02	kPa	Joback Method
rinpol	1102.00		NIST Webbook
tb	468.12	K	Joback Method
tc	679.14	K	Joback Method
tf	246.98	K	Joback Method
vc	0.483	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.43	J/mol×K	468.12	Joback Method
cpg	245.45	J/mol×K	503.29	Joback Method
cpg	255.83	J/mol×K	538.46	Joback Method
cpg	265.60	J/mol×K	573.63	Joback Method
cpg	274.79	J/mol×K	608.80	Joback Method
cpg	283.45	J/mol×K	643.97	Joback Method
cpg	291.59	J/mol×K	679.14	Joback Method
dvisc	0.0061816	Pa×s	246.98	Joback Method
dvisc	0.0027790	Pa×s	283.84	Joback Method

dvisc	0.0015014	Pa×s	320.69	Joback Method
dvisc	0.0009209	Pa×s	357.55	Joback Method
dvisc	0.0006189	Pa×s	394.41	Joback Method
dvisc	0.0004452	Pa×s	431.26	Joback Method
dvisc	0.0003373	Pa×s	468.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R294607&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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