

Pentane, 2,3-dibromo-, (R*,R*)-

Inchi:	InChI=1S/C5H10Br2/c1-3-5(7)4(2)6/h4-5H,3H2,1-2H3/t4-,5-/m0/s1
InchiKey:	LWBRXRHBXMVUEX-WHFBIAKZSA-N
Formula:	C5H10Br2
SMILES:	CCC(Br)C(C)Br
Mol. weight [g/mol]:	229.94
CAS:	22415-73-2

Physical Properties

Property code	Value	Unit	Source
gf	14.98	kJ/mol	Joback Method
hf	-104.43	kJ/mol	Joback Method
hfus	12.23	kJ/mol	Joback Method
hvap	38.82	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	2.943		Crippen Method
mcvol	116.310	ml/mol	McGowan Method
pc	4194.74	kPa	Joback Method
tb	445.24	K	Joback Method
tc	659.19	K	Joback Method
tf	235.71	K	Joback Method
vc	0.427	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	195.24	J/mol×K	445.24	Joback Method
cpg	238.42	J/mol×K	623.54	Joback Method
cpg	230.84	J/mol×K	587.88	Joback Method
cpg	222.76	J/mol×K	552.22	Joback Method
cpg	214.15	J/mol×K	516.56	Joback Method
cpg	204.99	J/mol×K	480.90	Joback Method
cpg	245.55	J/mol×K	659.19	Joback Method
dvisc	0.0003710	Pa×s	445.24	Joback Method
dvisc	0.0004872	Pa×s	410.32	Joback Method

dvisc	0.0006733	Pa×s	375.40	Joback Method
dvisc	0.0009942	Pa×s	340.48	Joback Method
dvisc	0.0016048	Pa×s	305.55	Joback Method
dvisc	0.0029311	Pa×s	270.63	Joback Method
dvisc	0.0063998	Pa×s	235.71	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22415732&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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