

Pentane, 2-bromo-2,4-dimethyl

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C7H15Br/c1-6(2)5-7(3,4)8/h6H,5H2,1-4H3

BKKLBSLWBNEGJL-UHFFFAOYSA-N

C7H15Br

CC(C)CC(C)(C)Br

179.10

Physical Properties

Property code	Value	Unit	Source
gf	22.78	kJ/mol	Joback Method
hf	-175.51	kJ/mol	Joback Method
hfus	8.23	kJ/mol	Joback Method
hvap	35.93	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	3.206		Crippen Method
mcvol	126.990	ml/mol	McGowan Method
pc	3107.10	kPa	Joback Method
rinpol	886.00		NIST Webbook
rinpol	886.00		NIST Webbook
tb	422.05	K	Joback Method
tc	621.29	K	Joback Method
tf	215.87	K	Joback Method
vc	0.472	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.44	J/mol×K	422.05	Joback Method
cpg	252.12	J/mol×K	455.26	Joback Method
cpg	265.00	J/mol×K	488.46	Joback Method
cpg	277.13	J/mol×K	521.67	Joback Method
cpg	288.54	J/mol×K	554.88	Joback Method
cpg	299.27	J/mol×K	588.08	Joback Method
cpg	309.36	J/mol×K	621.29	Joback Method
dvisc	0.0107490	Pa×s	215.87	Joback Method

dvisc	0.0040543	Pa×s	250.23	Joback Method
dvisc	0.0019352	Pa×s	284.60	Joback Method
dvisc	0.0010833	Pa×s	318.96	Joback Method
dvisc	0.0006789	Pa×s	353.32	Joback Method
dvisc	0.0004622	Pa×s	387.69	Joback Method
dvisc	0.0003350	Pa×s	422.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R597010&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

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