

Pentane, 3,3-bis(bromomethyl)-

Other names:	1,3-Dibromo-2,2-diethylpropane 3,3-bis(bromomethyl)pentane
Inchi:	InChI=1S/C7H14Br2/c1-3-7(4-2,5-8)6-9/h3-6H2,1-2H3
InchiKey:	ZIQNZEFIQWBNHV-UHFFFAOYSA-N
Formula:	C7H14Br2
SMILES:	CCC(CC)(CBr)CBr
Mol. weight [g/mol]:	257.99
CAS:	67969-84-0

Physical Properties

Property code	Value	Unit	Source
gf	39.54	kJ/mol	Joback Method
hf	-143.90	kJ/mol	Joback Method
hfus	17.04	kJ/mol	Joback Method
hvap	42.75	kJ/mol	Joback Method
log10ws	-3.37		Crippen Method
logp	3.583		Crippen Method
mvol	144.490	ml/mol	McGowan Method
pc	3329.68	kPa	Joback Method
tb	488.65	K	Joback Method
tc	700.57	K	Joback Method
tf	312.90 ± 2.00	K	NIST Webbook
vc	0.540	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.46	J/mol×K	488.65	Joback Method
cpg	290.97	J/mol×K	523.97	Joback Method
cpg	302.64	J/mol×K	559.29	Joback Method
cpg	313.52	J/mol×K	594.61	Joback Method
cpg	323.67	J/mol×K	629.93	Joback Method
cpg	333.15	J/mol×K	665.25	Joback Method
cpg	342.00	J/mol×K	700.57	Joback Method

dvisc	0.0039682	Paxs	290.67	Joback Method
dvisc	0.0021258	Paxs	323.67	Joback Method
dvisc	0.0012782	Paxs	356.66	Joback Method
dvisc	0.0008377	Paxs	389.66	Joback Method
dvisc	0.0005865	Paxs	422.66	Joback Method
dvisc	0.0004323	Paxs	455.65	Joback Method
dvisc	0.0003321	Paxs	488.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C67969840&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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