

2-Methyl-1,2-dibromopentane

Inchi:	InChI=1S/C6H12Br2/c1-3-4-6(2,8)5-7/h3-5H2,1-2H3
InchiKey:	JNWPBSNRFLWBNI-UHFFFAOYSA-N
Formula:	C6H12Br2
SMILES:	CCCC(C)(Br)CBr
Mol. weight [g/mol]:	243.97

Physical Properties

Property code	Value	Unit	Source
gf	31.12	kJ/mol	Joback Method
hf	-123.26	kJ/mol	Joback Method
hfus	14.45	kJ/mol	Joback Method
hvap	40.52	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	3.335		Crippen Method
mcvol	130.400	ml/mol	McGowan Method
pc	3731.66	kPa	Joback Method
rinpol	1059.00		NIST Webbook
rinpol	1091.00		NIST Webbook
tb	465.77	K	Joback Method
tc	680.86	K	Joback Method
tf	279.40	K	Joback Method
vc	0.484	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	237.14	J/molxK	465.77	Joback Method
cpg	248.60	J/molxK	501.62	Joback Method
cpg	259.25	J/molxK	537.47	Joback Method
cpg	269.14	J/molxK	573.31	Joback Method
cpg	278.32	J/molxK	609.16	Joback Method
cpg	286.87	J/molxK	645.01	Joback Method
cpg	294.82	J/molxK	680.86	Joback Method
dvisc	0.0041844	Paxs	279.40	Joback Method

dvisc	0.0022883	Paxs	310.46	Joback Method
dvisc	0.0013966	Paxs	341.52	Joback Method
dvisc	0.0009255	Paxs	372.58	Joback Method
dvisc	0.0006534	Paxs	403.65	Joback Method
dvisc	0.0004849	Paxs	434.71	Joback Method
dvisc	0.0003744	Paxs	465.77	Joback Method

Sources

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=R559281&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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