

1-Allyl-3-methylbenzene

Inchi:	InChI=1S/C7H11Br/c1-6-2-4-7(8)5-3-6/h4,6H,2-3,5H2,1H3
InchiKey:	LIUFYLLBQSSKQS-UHFFFAOYSA-N
Formula:	C7H11Br
SMILES:	CC1CC=C(Br)CC1
Mol. weight [g/mol]:	175.07

Physical Properties

Property code	Value	Unit	Source
gf	67.16	kJ/mol	Joback Method
hf	-60.85	kJ/mol	Joback Method
hfus	11.84	kJ/mol	Joback Method
hvap	38.99	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	3.085		Crippen Method
mcvol	111.830	ml/mol	McGowan Method
pc	3930.78	kPa	Joback Method
rinpol	1028.00		NIST Webbook
rinpol	1029.00		NIST Webbook
rinpol	1028.00		NIST Webbook
tb	449.41	K	Joback Method
tc	676.42	K	Joback Method
tf	249.11	K	Joback Method
vc	0.408	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.76	J/molxK	449.41	Joback Method
cpg	266.46	J/molxK	638.59	Joback Method
cpg	255.46	J/molxK	600.75	Joback Method
cpg	243.72	J/molxK	562.92	Joback Method
cpg	231.21	J/molxK	525.08	Joback Method
cpg	217.90	J/molxK	487.25	Joback Method
cpg	276.75	J/molxK	676.42	Joback Method

dvisc	0.0003401	Paxs	449.41	Joback Method
dvisc	0.0004237	Paxs	416.03	Joback Method
dvisc	0.0005486	Paxs	382.64	Joback Method
dvisc	0.0007462	Paxs	349.26	Joback Method
dvisc	0.0010832	Paxs	315.88	Joback Method
dvisc	0.0017171	Paxs	282.49	Joback Method
dvisc	0.0030799	Paxs	249.11	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=R594888&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
mvol:	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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