

Allyl dibromoacetate

Inchi:	InChI=1S/C5H6Br2O2/c1-2-3-9-5(8)4(6)7/h2,4H,1,3H2
InchiKey:	BQKSBGWDSUKUDU-UHFFFAOYSA-N
Formula:	C5H6Br2O2
SMILES:	C=CCOC(=O)C(Br)Br
Mol. weight [g/mol]:	257.91

Physical Properties

Property code	Value	Unit	Source
gf	-128.66	kJ/mol	Joback Method
hf	-218.52	kJ/mol	Joback Method
hfus	17.26	kJ/mol	Joback Method
hvap	47.69	kJ/mol	Joback Method
log10ws	-2.10		Crippen Method
logp	1.831		Crippen Method
mcvol	119.450	ml/mol	McGowan Method
pc	4665.71	kPa	Joback Method
rinpola	1114.00		NIST Webbook
ripola	1742.00		NIST Webbook
tb	518.65	K	Joback Method
tc	740.81	K	Joback Method
tf	321.11	K	Joback Method
vc	0.439	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	208.65	J/molxK	518.65	Joback Method
cpg	216.10	J/molxK	555.68	Joback Method
cpg	223.09	J/molxK	592.70	Joback Method
cpg	229.63	J/molxK	629.73	Joback Method
cpg	235.74	J/molxK	666.75	Joback Method
cpg	241.44	J/molxK	703.78	Joback Method
cpg	246.76	J/molxK	740.81	Joback Method
dvisc	0.0025137	Paxs	321.11	Joback Method

dvisc	0.0015401	Paxs	354.03	Joback Method
dvisc	0.0010256	Paxs	386.96	Joback Method
dvisc	0.0007279	Paxs	419.88	Joback Method
dvisc	0.0005431	Paxs	452.80	Joback Method
dvisc	0.0004216	Paxs	485.73	Joback Method
dvisc	0.0003380	Paxs	518.65	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R26617&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

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

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