

Amyl-2,4-dibromophenyl ether

Inchi:	InChI=1S/C11H14Br2O/c1-2-3-4-7-14-11-6-5-9(12)8-10(11)13/h5-6,8H,2-4,7H2,1H3
InchiKey:	BWTNJRCDYGLTRF-UHFFFAOYSA-N
Formula:	C11H14Br2O
SMILES:	CCCCCOc1ccc(Br)cc1Br
Mol. weight [g/mol]:	322.04
CAS:	63076-62-0

Physical Properties

Property code	Value	Unit	Source
gf	58.53	kJ/mol	Joback Method
hf	-136.34	kJ/mol	Joback Method
hfus	29.27	kJ/mol	Joback Method
hvap	58.96	kJ/mol	Joback Method
log10ws	-5.59		Crippen Method
logp	4.781		Crippen Method
mcvol	182.960	ml/mol	McGowan Method
pc	2915.53	kPa	Joback Method
tb	642.46	K	Joback Method
tc	871.32	K	Joback Method
tf	407.02	K	Joback Method
vc	0.685	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	405.65	J/molxK	642.46	Joback Method
cpg	418.65	J/molxK	680.60	Joback Method
cpg	430.83	J/molxK	718.75	Joback Method
cpg	442.23	J/molxK	756.89	Joback Method
cpg	452.88	J/molxK	795.04	Joback Method
cpg	462.82	J/molxK	833.18	Joback Method
cpg	472.09	J/molxK	871.32	Joback Method
dvisc	0.0009709	Paxs	407.02	Joback Method
dvisc	0.0006345	Paxs	446.26	Joback Method

dvisc	0.0004442	Paxs	485.50	Joback Method
dvisc	0.0003280	Paxs	524.74	Joback Method
dvisc	0.0002526	Paxs	563.98	Joback Method
dvisc	0.0002013	Paxs	603.22	Joback Method
dvisc	0.0001649	Paxs	642.46	Joback Method

Sources

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=C63076620&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mccvol:	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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