

4-Bromo-o-toloxxy acetic acid

Inchi:	InChI=1S/C9H9BrO3/c1-6-2-3-7(10)4-8(6)13-5-9(11)12/h2-4H,5H2,1H3,(H,11,12)
InchiKey:	KQQHLMBLDZPBCO-UHFFFAOYSA-N
Formula:	C9H9BrO3
SMILES:	Cc1ccc(Br)cc1OCC(=O)O
Mol. weight [g/mol]:	245.07
CAS:	25477-00-3

Physical Properties

Property code	Value	Unit	Source
gf	-238.37	kJ/mol	Joback Method
hf	-386.20	kJ/mol	Joback Method
hfus	24.49	kJ/mol	Joback Method
hvap	71.50	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	2.221		Crippen Method
mcvol	144.720	ml/mol	McGowan Method
pc	4036.37	kPa	Joback Method
tb	676.59	K	Joback Method
tc	891.07	K	Joback Method
tf	435.43	K	Joback Method
vc	0.536	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.69	J/mol×K	676.59	Joback Method
cpg	372.02	J/mol×K	855.32	Joback Method
cpg	365.25	J/mol×K	819.58	Joback Method
cpg	357.94	J/mol×K	783.83	Joback Method
cpg	350.09	J/mol×K	748.08	Joback Method
cpg	341.68	J/mol×K	712.34	Joback Method
cpg	378.28	J/mol×K	891.07	Joback Method
dvisc	0.0000611	Pa×s	676.59	Joback Method
dvisc	0.0000844	Pa×s	636.40	Joback Method

dvisc	0.0001217	Pa×s	596.20	Joback Method
dvisc	0.0001852	Pa×s	556.01	Joback Method
dvisc	0.0003009	Pa×s	515.82	Joback Method
dvisc	0.0005305	Pa×s	475.62	Joback Method
dvisc	0.0010385	Pa×s	435.43	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25477003&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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