4-Bromobenzoic acid, 3-chloroprop-2-enyl ester

Inchi: InChI=1S/C10H8BrClO2/c11-9-4-2-8(3-5-9)10(13)14-7-1-6-12/h1-6H,7H2/b6-1+

InchiKey: OKPLUDOVIAXINL-LZCJLJQNSA-N

Formula: C10H8BrClO2

SMILES: O=C(OCC=CCl)c1ccc(Br)cc1

Mol. weight [g/mol]: 275.53

Physical Properties

Property code	Value	Unit	Source
gf	-15.21	kJ/mol	Joback Method
hf	-141.66	kJ/mol	Joback Method
hfus	27.78	kJ/mol	Joback Method
hvap	60.73	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	3.358		Crippen Method
mcvol	160.880	ml/mol	McGowan Method
pc	3333.53	kPa	Joback Method
rinpol	1704.00		NIST Webbook
rinpol	1704.00		NIST Webbook
tb	643.90	K	Joback Method
tc	884.33	K	Joback Method
tf	398.20	K	Joback Method
vc	0.603	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.32	J/mol×K	643.90	Joback Method
cpg	348.89	J/mol×K	683.97	Joback Method
cpg	358.65	J/mol×K	724.04	Joback Method
cpg	367.64	J/mol×K	764.12	Joback Method
cpg	375.93	J/mol×K	804.19	Joback Method
cpg	383.56	J/mol×K	844.26	Joback Method
cpg	390.58	J/mol×K	884.33	Joback Method
dvisc	0.0011966	Pa×s	398.20	Joback Method

dvisc	0.0007430	Pa×s	439.15	Joback Method
dvisc	0.0005005	Pa×s	480.10	Joback Method
dvisc	0.0003587	Pa×s	521.05	Joback Method
dvisc	0.0002699	Pa×s	562.00	Joback Method
dvisc	0.0002110	Pa×s	602.95	Joback Method
dvisc	0.0001703	Pa×s	643.90	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U299253&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

rinpol: Non-polar retention indices

tb: Normal Boiling Point Temperature

tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume