1-(2-Bromoethoxy)-2,4-dichlorobenzene

Inchi: InChI=1S/C8H7BrCl2O/c9-3-4-12-8-2-1-6(10)5-7(8)11/h1-2,5H,3-4H2
InchiKey: OEYZGSRLAGSENP-UHFFFAOYSA-N
Formula: C8H7BrCl2O
SMILES: Clc1ccc(OCCBr)c(Cl)c1
Mol. weight [g/mol]: 269.95
CAS: 6954-77-4

Physical Properties

Property code	Value	Unit	Source
gf	-4.91	kJ/mol	Joback Method
hf	-132.23	kJ/mol	Joback Method
hfus	24.61	kJ/mol	Joback Method
hvap	54.62	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.767		Crippen Method
mcvol	147.670	ml/mol	McGowan Method
pc	3431.89	kPa	Joback Method
tb	582.52	K	Joback Method
tc	819.91	K	Joback Method
tf	373.25	K	Joback Method
vc	0.553	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.96	J/mol×K	582.52	Joback Method
cpg	288.59	J/mol×K	622.09	Joback Method
cpg	297.59	J/mol×K	661.65	Joback Method
cpg	305.97	J/mol×K	701.22	Joback Method
cpg	313.76	J/mol×K	740.78	Joback Method
cpg	320.97	J/mol×K	780.35	Joback Method
cpg	327.63	J/mol×K	819.91	Joback Method
dvisc	0.0011698	Pa×s	373.25	Joback Method
dvisc	0.0007847	Pa×s	408.13	Joback Method

dvisc	0.0005605	Pa×s	443.01	Joback Method
dvisc	0.0004205	Pa×s	477.88	Joback Method
dvisc	0.0003281	Pa×s	512.76	Joback Method
dvisc	0.0002642	Pa×s	547.64	Joback Method
dvisc	0.0002183	Pa×s	582.52	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	446.50 ± 1.50	K	2.40	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6954774&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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume