2,3-Difluorobenzyl bromide

Inchi: InChI=1S/C7H5BrF2/c8-4-5-2-1-3-6(9)7(5)10/h1-3H,4H2
InchiKey: FTBSGSZZESQDBM-UHFFFAOYSA-N
Formula: C7H5BrF2
SMILES: Fc1cccc(CBr)c1F
Mol. weight [g/mol]: 207.01
CAS: 113211-94-2

Physical Properties

Property code	Value	Unit	Source
gf	-274.09	kJ/mol	Joback Method
hf	-340.11	kJ/mol	Joback Method
hfus	18.59	kJ/mol	Joback Method
hvap	39.58	kJ/mol	Joback Method
log10ws	-3.45		Crippen Method
logp	2.860		Crippen Method
mcvol	106.770	ml/mol	McGowan Method
pc	3857.88	kPa	Joback Method
tb	460.90	K	Joback Method
tc	671.11	K	Joback Method
tf	281.09	K	Joback Method
vc	0.417	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	190.11	J/mol×K	460.90	Joback Method
cpg	199.00	J/mol×K	495.93	Joback Method
cpg	207.35	J/mol×K	530.97	Joback Method
cpg	215.19	J/mol×K	566.00	Joback Method
cpg	222.54	J/mol×K	601.04	Joback Method
cpg	229.41	J/mol×K	636.07	Joback Method
cpg	235.85	J/mol×K	671.11	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=C113211942&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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

Latest version available from:
https://www.chemeo.com/cid/10-029-8/2-3-Difluorobenzyl-bromide.pdf
Generated by Cheméo on 2024-04-17 15:58:10.341315273 +0000 UTC m=+15658739.261892588.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.