2,6-Diethylbromobenzene

Other names: 1-Bromo-2,6-diethylbenzene
Benzene, 2-bromo-1,3-diethyl-
Inchi: InChI=1S/C10H13Br/c1-3-8-6-5-7-9(4-2)10(8)11/h5-7H,3-4H2,1-2H3
InchiKey: FPWGIABDOFXETH-UHFFFAOYSA-N
Formula: C10H13Br
SMILES: CCc1cccc(CC)c1Br
Mol. weight [g/mol]: 213.11
CAS: 65232-57-7

Physical Properties

Property code	Value	Unit	Source
gf	140.79	kJ/mol	Joback Method
hf	-9.81	kJ/mol	Joback Method
hfus	20.20	kJ/mol	Joback Method
hvap	47.89	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	3.574		Crippen Method
mcvol	145.500	ml/mol	McGowan Method
pc	3059.17	kPa	Joback Method
tb	531.00	K	Joback Method
tc	754.14	K	Joback Method
tf	313.72	K	Joback Method
vc	0.549	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.18	J/mol×K	531.00	Joback Method
cpg	311.70	J/mol×K	568.19	Joback Method
cpg	324.42	J/mol×K	605.38	Joback Method
cpg	336.38	J/mol×K	642.57	Joback Method
cpg	347.62	J/mol×K	679.76	Joback Method
cpg	358.17	J/mol×K	716.95	Joback Method
cpg	368.07	J/mol×K	754.14	Joback Method

dvisc	0.0016521	Pa×s	313.72	Joback Method
dvisc	0.0010180	Pa×s	349.93	Joback Method
dvisc	0.0006870	Pa×s	386.15	Joback Method
dvisc	0.0004959	Pa×s	422.36	Joback Method
dvisc	0.0003769	Pa×s	458.57	Joback Method
dvisc	0.0002982	Pa×s	494.79	Joback Method
dvisc	0.0002436	Pa×s	531.00	Joback Method

Sources

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=C65232577&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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