Phenetole: beta-bromo-2,3,4,5,6-pentafluoro-

Inchi: InChI=1S/C8H4BrF5O/c9-1-2-15-8-6(13)4(11)3(10)5(12)7(8)14/h1-2H2
InchiKey: DZKOVQHPLXTXML-UHFFFAOYSA-N
Formula: C8H4BrF5O
SMILES: Fc1c(F)c(F)c(OCCBr)c(F)c1F
Mol. weight [g/mol]: 291.01
CAS: 6669-01-8

Physical Properties

Property code	Value	Unit	Source
gf	-983.99	kJ/mol	Joback Method
hf	-1115.71	kJ/mol	Joback Method
hfus	30.45	kJ/mol	Joback Method
hvap	43.75	kJ/mol	Joback Method
log10ws	-4.10		Crippen Method
logp	3.156		Crippen Method
mcvol	132.040	ml/mol	McGowan Method
pc	2761.36	kPa	Joback Method
tb	518.95	K	Joback Method
tc	699.29	K	Joback Method
tf	353.92	K	Joback Method
vc	0.545	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	274.62	J/mol×K	518.95	Joback Method
cpg	282.28	J/mol×K	549.01	Joback Method
cpg	289.64	J/mol×K	579.06	Joback Method
cpg	296.71	J/mol×K	609.12	Joback Method
cpg	303.49	J/mol×K	639.17	Joback Method
cpg	309.97	J/mol×K	669.23	Joback Method
cpg	316.15	J/mol×K	699.29	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=C6669018&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
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