Halfenprox

Other names: Benzene, 1-[[2-[4-(bromodifluoromethoxy)phenyl]-2-methylpropoxy]methyl]-3-phenoxy-
Inchi: InChI=1S/C24H23BrF2O3/c1-23(2,19-11-13-21(14-12-19)30-24(25,26)27)17-28-16-18-7-
InchiKey: WIFXJBMOTMKRMM-UHFFFAOYSA-N
Formula: C24H23BrF2O3
SMILES: CC(C)(COCc1cccc(Oc2ccccc2)c1)c1ccc(OC(F)(F)Br)cc1
Mol. weight [g/mol]: 477.34
CAS: 111872-58-3

Physical Properties

Property code	Value	Unit	Source
gf	-215.45	kJ/mol	Joback Method
hf	-632.09	kJ/mol	Joback Method
hfus	39.44	kJ/mol	Joback Method
hvap	86.61	kJ/mol	Joback Method
log10ws	-7.89		Crippen Method
logp	7.297		Crippen Method
mcvol	316.390	ml/mol	McGowan Method
pc	1487.29	kPa	Joback Method
rinpol	2841.00		NIST Webbook
rinpol	2841.00		NIST Webbook
tb	964.02	K	Joback Method
tc	1208.87	K	Joback Method
tf	597.05	K	Joback Method
vc	1.185	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	965.59	J/mol×K	964.02	Joback Method
cpg	979.02	J/mol×K	1004.83	Joback Method
cpg	991.22	J/mol×K	1045.64	Joback Method
cpg	1002.29	J/mol×K	1086.44	Joback Method
cpg	1012.39	J/mol×K	1127.25	Joback Method
cpg	1021.64	J/mol×K	1168.06	Joback Method

cpg	1030.18	J/mol×K	1208.87	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C111872583&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume