1-(8-Bromo-2,3,6,7-tetrahydrodibenzo[1,2-b;4,5-b']difuran-4-yl-2-aminopropane, N-methyl, TFA

InChI: InChI=1S/C16H17BrF3NO3/c1-8(21(2)15(22)16(18,19)20)7-11-9-3-5-24-14(9)12(17)10-4

InchiKey: UBHPWSSCACYUJZ-UHFFFAOYSA-N

Formula: C16H17BrF3NO3

SMILES: CC(Cc1c2c(c(Br)c3c1OCC3)OCC2)N(C)C(=O)C(F)(F)F

Mol. weight [g/mol]: 408.21

Physical Properties

Property code	Value	Unit	Source
gf	-475.07	kJ/mol	Joback Method
hf	-893.19	kJ/mol	Joback Method
hfus	47.59	kJ/mol	Joback Method
hvap	77.35	kJ/mol	Joback Method
log10ws	-5.03		Crippen Method
logp	3.271		Crippen Method
mcvol	236.920	ml/mol	McGowan Method
pc	2127.56	kPa	Joback Method
rinpol	2380.00		NIST Webbook
rinpol	2336.00		NIST Webbook
rinpol	2336.00		NIST Webbook
tb	820.39	K	Joback Method
tc	1039.19	K	Joback Method
tf	587.99	K	Joback Method
vc	0.904	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	698.85	J/mol×K	820.39	Joback Method
cpg	711.42	J/mol×K	856.86	Joback Method
cpg	723.32	J/mol×K	893.32	Joback Method
cpg	734.69	J/mol×K	929.79	Joback Method
cpg	745.67	J/mol×K	966.26	Joback Method
cpg	756.39	J/mol×K	1002.73	Joback Method
cpg	766.98	J/mol×K	1039.19	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=R640505&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume