Succinic acid, 2-bromo-4-fluorophenyl 2-(dimethylamino)ethyl ester

Inchi: InChI=1S/C14H17BrFNO4/c1-17(2)7-8-20-13(18)5-6-14(19)21-12-4-3-10(16)9-11(12)15/

InchiKey: HQTSAVZVFVQKCZ-UHFFFAOYSA-N

Formula: C14H17BrFNO4

SMILES: CN(C)CCOC(=O)CCC(=O)Oc1ccc(F)cc1Br

Mol. weight [g/mol]: 362.19

Physical Properties

Property code	Value	Unit	Source
gf	-377.40	kJ/mol	Joback Method
hf	-710.55	kJ/mol	Joback Method
hfus	42.24	kJ/mol	Joback Method
hvap	76.33	kJ/mol	Joback Method
log10ws	-3.22		Crippen Method
logp	2.379		Crippen Method
mcvol	228.490	ml/mol	McGowan Method
pc	2169.38	kPa	Joback Method
rinpol	2203.00		NIST Webbook
rinpol	2203.00		NIST Webbook
tb	786.81	K	Joback Method
tc	994.56	K	Joback Method
tf	536.18	K	Joback Method
vc	0.858	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	623.93	J/mol×K	786.81	Joback Method
cpg	636.31	J/mol×K	821.44	Joback Method
cpg	647.78	J/mol×K	856.06	Joback Method
cpg	658.37	J/mol×K	890.69	Joback Method
cpg	668.09	J/mol×K	925.31	Joback Method
cpg	676.96	J/mol×K	959.94	Joback Method
cpg	685.01	J/mol×K	994.56	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=U358014&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume