Succinic acid, 2-bromo-4-fluorophenyl N,N-diethyl-2-aminoethyl ester

Inchi: InChI=1S/C16H21BrFNO4/c1-3-19(4-2)9-10-22-15(20)7-8-16(21)23-14-6-5-12(18)11-13(

InchiKey: JRNLMGWRMWEWQJ-UHFFFAOYSA-N

Formula: C16H21BrFNO4

SMILES: CCN(CC)CCOC(=O)CCC(=O)Oc1ccc(F)cc1Br

Mol. weight [g/mol]: 390.25

Physical Properties

Property code	Value	Unit	Source
gf	-360.56	kJ/mol	Joback Method
hf	-751.83	kJ/mol	Joback Method
hfus	47.42	kJ/mol	Joback Method
hvap	80.78	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.159		Crippen Method
mcvol	256.670	ml/mol	McGowan Method
pc	1827.85	kPa	Joback Method
rinpol	2373.00		NIST Webbook
tb	832.57	K	Joback Method
tc	1038.38	K	Joback Method
tf	558.72	K	Joback Method
vc	0.970	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	734.78	J/mol×K	832.57	Joback Method
cpg	747.81	J/mol×K	866.87	Joback Method
cpg	759.86	J/mol×K	901.17	Joback Method
cpg	770.97	J/mol×K	935.47	Joback Method
cpg	781.16	J/mol×K	969.77	Joback Method
cpg	790.44	J/mol×K	1004.08	Joback Method
cpg	798.86	J/mol×K	1038.38	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=U358020&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