Succinic acid, butyl 4-fluoro-3-nitrobenzyl ester

Inchi: InChI=1S/C15H18FNO6/c1-2-3-8-22-14(18)6-7-15(19)23-10-11-4-5-12(16)13(9-11)17(20

InchiKey: KWECPRPYJKFPFS-UHFFFAOYSA-N

Formula: C15H18FNO6

SMILES: CCCCOC(=O)CCC(=O)OCc1ccc(F)c([N+](=O)[O-])c1

Mol. weight [g/mol]: 327.30

Physical Properties

Property code	Value	Unit	Source
gf	-458.53	kJ/mol	Joback Method
hf	-835.81	kJ/mol	Joback Method
hfus	47.88	kJ/mol	Joback Method
hvap	86.67	kJ/mol	Joback Method
log10ws	-4.41		Crippen Method
logp	2.901		Crippen Method
mcvol	232.520	ml/mol	McGowan Method
pc	1893.65	kPa	Joback Method
rinpol	2352.00		NIST Webbook
rinpol	2352.00		NIST Webbook
tb	882.93	K	Joback Method
tc	1101.39	K	Joback Method
tf	598.79	K	Joback Method
vc	0.915	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	704.14	J/mol×K	882.93	Joback Method
cpg	715.54	J/mol×K	919.34	Joback Method
cpg	725.85	J/mol×K	955.75	Joback Method
cpg	735.08	J/mol×K	992.16	Joback Method
cpg	743.24	J/mol×K	1028.57	Joback Method
cpg	750.34	J/mol×K	1064.98	Joback Method
cpg	756.39	J/mol×K	1101.39	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381018&Units=SI
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

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

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