

Succinic acid, 2-fluoro-5-nitrobenzyl isobutyl ester

Inchi:	InChI=1S/C15H18FNO6/c1-10(2)8-22-14(18)5-6-15(19)23-9-11-7-12(17(20)21)3-4-13(11)
InchiKey:	WDEMZHJCHTYCBY-UHFFFAOYSA-N
Formula:	C15H18FNO6
SMILES:	CC(C)COC(=O)CCC(=O)OCc1cc([N+](=O)[O-])ccc1F
Mol. weight [g/mol]:	327.30

Physical Properties

Property code	Value	Unit	Source
gf	-460.97	kJ/mol	Joback Method
hf	-841.09	kJ/mol	Joback Method
hfus	44.36	kJ/mol	Joback Method
hvap	86.28	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	2.756		Crippen Method
mvol	232.520	ml/mol	McGowan Method
pc	1906.90	kPa	Joback Method
rinpol	2275.00		NIST Webbook
rinpol	2275.00		NIST Webbook
tb	882.49	K	Joback Method
tc	1103.39	K	Joback Method
tf	583.79	K	Joback Method
vc	0.909	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	704.70	J/molxK	882.49	Joback Method
cpg	716.20	J/molxK	919.31	Joback Method
cpg	726.57	J/molxK	956.12	Joback Method
cpg	735.82	J/molxK	992.94	Joback Method
cpg	743.96	J/molxK	1029.75	Joback Method
cpg	751.01	J/molxK	1066.57	Joback Method
cpg	756.98	J/molxK	1103.39	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=U380924&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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