

Succinic acid, di(5-fluoro-2-nitrophenyl) ester

Inchi:	InChI=1S/C16H10F2N2O8/c17-9-1-3-11(19(23)24)13(7-9)27-15(21)5-6-16(22)28-14-8-10
InchiKey:	AWJISDLCZOVTBA-UHFFFAOYSA-N
Formula:	C16H10F2N2O8
SMILES:	O=C(CCC(=O)Oc1cc(F)ccc1[N+](=O)[O-])Oc1cc(F)ccc1[N+](=O)[O-]
Mol. weight [g/mol]:	396.26

Physical Properties

Property code	Value	Unit	Source
gf	-516.22	kJ/mol	Joback Method
hf	-849.73	kJ/mol	Joback Method
hfus	58.18	kJ/mol	Joback Method
hvap	108.27	kJ/mol	Joback Method
log10ws	-5.71		Crippen Method
logp	3.072		Crippen Method
mvol	242.040	ml/mol	McGowan Method
pc	2212.45	kPa	Joback Method
rinpol	2877.00		NIST Webbook
tb	1093.56	K	Joback Method
tc	1352.38	K	Joback Method
tf	805.72	K	Joback Method
vc	0.964	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	731.16	J/molxK	1093.56	Joback Method
cpg	735.25	J/molxK	1136.70	Joback Method
cpg	737.90	J/molxK	1179.83	Joback Method
cpg	739.13	J/molxK	1222.97	Joback Method
cpg	738.96	J/molxK	1266.11	Joback Method
cpg	737.43	J/molxK	1309.25	Joback Method
cpg	734.56	J/molxK	1352.38	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=U357985&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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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