

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

Inchi:	InChI=1S/C20H28FNO6/c1-2-3-4-5-6-7-8-13-27-19(23)11-12-20(24)28-15-16-14-17(22)(2)
InchiKey:	NSYAVVPSZKYODL-UHFFFAOYSA-N
Formula:	C20H28FNO6
SMILES:	CCCCCCCCCOC(=O)CCC(=O)OCc1cc([N+](=O)[O-])ccc1F
Mol. weight [g/mol]:	397.44

Physical Properties

Property code	Value	Unit	Source
gf	-416.43	kJ/mol	Joback Method
hf	-939.01	kJ/mol	Joback Method
hfus	60.83	kJ/mol	Joback Method
hvap	97.80	kJ/mol	Joback Method
log10ws	-6.50		Crippen Method
logp	4.851		Crippen Method
mvol	302.970	ml/mol	McGowan Method
pc	1295.79	kPa	Joback Method
rinpol	2821.00		NIST Webbook
rinpol	2821.00		NIST Webbook
tb	997.33	K	Joback Method
tc	1222.24	K	Joback Method
tf	655.14	K	Joback Method
vc	1.196	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	993.96	J/molxK	997.33	Joback Method
cpg	1006.19	J/molxK	1034.81	Joback Method
cpg	1017.04	J/molxK	1072.30	Joback Method
cpg	1026.57	J/molxK	1109.78	Joback Method
cpg	1034.79	J/molxK	1147.27	Joback Method
cpg	1041.75	J/molxK	1184.75	Joback Method
cpg	1047.46	J/molxK	1222.24	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U380931&Units=SI

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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