

Succinic acid, di(2,3,6-trifluorobenzyl) ester

Inchi: InChI=1S/C18H12F6O4/c19-11-1-3-13(21)17(23)9(11)7-27-15(25)5-6-16(26)28-8-10-12(20)
InchiKey: NTRVJVBABTJ-UHFFFAOYSA-N
Formula: C18H12F6O4
SMILES: O=C(CCC(=O)OCc1c(F)ccc(F)c1F)OCc1c(F)ccc(F)c1F
Mol. weight [g/mol]: 406.28

Physical Properties

Property code	Value	Unit	Source
gf	-1368.98	kJ/mol	Joback Method
hf	-1676.87	kJ/mol	Joback Method
hfus	52.18	kJ/mol	Joback Method
hvap	77.60	kJ/mol	Joback Method
log10ws	-6.27		Crippen Method
logp	4.088		Crippen Method
mvol	242.460	ml/mol	McGowan Method
pc	1535.46	kPa	Joback Method
rinpol	2302.00		NIST Webbook
rinpol	2302.00		NIST Webbook
tb	842.68	K	Joback Method
tc	1040.56	K	Joback Method
tf	568.44	K	Joback Method
vc	0.984	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	706.61	J/molxK	842.68	Joback Method
cpg	717.48	J/molxK	875.66	Joback Method
cpg	727.42	J/molxK	908.64	Joback Method
cpg	736.44	J/molxK	941.62	Joback Method
cpg	744.53	J/molxK	974.60	Joback Method
cpg	751.70	J/molxK	1007.58	Joback Method
cpg	757.95	J/molxK	1040.56	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=U381190&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
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
rlnol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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