

Succinic acid, ethyl 3,4,5-trifluorobenzyl ester

Inchi: InChI=1S/C13H13F3O4/c1-2-19-11(17)3-4-12(18)20-7-8-5-9(14)13(16)10(15)6-8/h5-6H,1-4H3
InchiKey: ZDIJEZOAJSJDDJ-UHFFFAOYSA-N
Formula: C13H13F3O4
SMILES: CCOC(=O)CCC(=O)OCc1cc(F)c(F)c(F)c1
Mol. weight [g/mol]: 290.24

Physical Properties

Property code	Value	Unit	Source
gf	-910.17	kJ/mol	Joback Method
hf	-1187.46	kJ/mol	Joback Method
hfus	37.11	kJ/mol	Joback Method
hvap	64.66	kJ/mol	Joback Method
log10ws	-3.58		Crippen Method
logp	2.490		Crippen Method
mvol	190.460	ml/mol	McGowan Method
pc	2023.58	kPa	Joback Method
rinpol	1710.00		NIST Webbook
rinpol	1710.00		NIST Webbook
tb	688.85	K	Joback Method
tc	876.71	K	Joback Method
tf	446.34	K	Joback Method
vc	0.757	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	509.51	J/molxK	688.85	Joback Method
cpg	521.49	J/molxK	720.16	Joback Method
cpg	532.79	J/molxK	751.47	Joback Method
cpg	543.44	J/molxK	782.78	Joback Method
cpg	553.40	J/molxK	814.09	Joback Method
cpg	562.70	J/molxK	845.40	Joback Method
cpg	571.32	J/molxK	876.71	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382184&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
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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