

Succinic acid, heptyl 4-trifluoromethylbenzyl ester

Inchi:	InChI=1S/C19H25F3O4/c1-2-3-4-5-6-13-25-17(23)11-12-18(24)26-14-15-7-9-16(10-8-15
InchiKey:	ZYLLVCNOFLIJHN-UHFFFAOYSA-N
Formula:	C19H25F3O4
SMILES:	CCCCCCCOC(=O)CCC(=O)OCc1ccc(C(F)(F)F)cc1
Mol. weight [g/mol]:	374.39

Physical Properties

Property code	Value	Unit	Source
gf	-837.55	kJ/mol	Joback Method
hf	-1297.11	kJ/mol	Joback Method
hfus	46.02	kJ/mol	Joback Method
hvap	75.39	kJ/mol	Joback Method
log10ws	-5.78		Crippen Method
logp	5.042		Crippen Method
mvol	275.000	ml/mol	McGowan Method
pc	1322.31	kPa	Joback Method
rinpol	2211.00		NIST Webbook
rinpol	2211.00		NIST Webbook
tb	812.94	K	Joback Method
tc	1004.64	K	Joback Method
tf	491.34	K	Joback Method
vc	1.083	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	842.80	J/molxK	812.94	Joback Method
cpg	857.56	J/molxK	844.89	Joback Method
cpg	871.33	J/molxK	876.84	Joback Method
cpg	884.14	J/molxK	908.79	Joback Method
cpg	896.01	J/molxK	940.74	Joback Method
cpg	907.00	J/molxK	972.69	Joback Method
cpg	917.13	J/molxK	1004.64	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=U382445&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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