Succinic acid, heptyl 2-(trifluoromethyl)benzyl ester

Inchi: InChI=1S/C19H25F3O4/c1-2-3-4-5-8-13-25-17(23)11-12-18(24)26-14-15-9-6-7-10-16(15

InchiKey: WFDQWKZYHYRTSP-UHFFFAOYSA-N

Formula: C19H25F3O4

SMILES: CCCCCCCOC(=O)CCC(=O)OCc1ccccc1C(F)(F)F

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
mcvol	275.000	ml/mol	McGowan Method
pc	1322.31	kPa	Joback Method
rinpol	2220.00		NIST Webbook
rinpol	2220.00		NIST Webbook
tb	812.94	K	Joback Method
tc	1004.64	K	Joback Method
tf	491.34	K	Joback Method
vc	1.083	m3/kmol	Joback Method

Temperature Dependent Properties

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

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381656&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
hvap:	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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume