Succinic acid, cyclohexylmethyl 2-fluoro-3-(trifluoromethyl)phenyl ester

Inchi: InChI=1S/C18H20F4O4/c19-17-13(18(20,21)22)7-4-8-14(17)26-16(24)10-9-15(23)25-11-

InchiKey: YHLUDQLVMLUCSE-UHFFFAOYSA-N

Formula: C18H20F4O4

SMILES: O=C(CCC(=O)Oc1cccc(C(F)(F)F)c1F)OCC1CCCCC1

Mol. weight [g/mol]: 376.34

Physical Properties

Property code	Value	Unit	Source
gf	-1025.96	kJ/mol	Joback Method
hf	-1429.73	kJ/mol	Joback Method
hfus	37.95	kJ/mol	Joback Method
hvap	73.44	kJ/mol	Joback Method
log10ws	-5.50		Crippen Method
logp	4.654		Crippen Method
mcvol	251.820	ml/mol	McGowan Method
pc	1588.54	kPa	Joback Method
tb	813.86	K	Joback Method
tc	1019.27	K	Joback Method
tf	500.56	K	Joback Method
vc	0.978	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	786.43	J/mol×K	813.86	Joback Method
cpg	801.31	J/mol×K	848.10	Joback Method
cpg	814.98	J/mol×K	882.33	Joback Method
cpg	827.47	J/mol×K	916.57	Joback Method
cpg	838.82	J/mol×K	950.80	Joback Method
cpg	849.08	J/mol×K	985.04	Joback Method
cpg	858.27	J/mol×K	1019.27	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390786&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume