Succinic acid, heptyl 2,3,6-trifluorobenzyl ester

Inchi: InChI=1S/C18H23F3O4/c1-2-3-4-5-6-11-24-16(22)9-10-17(23)25-12-13-14(19)7-8-15(20

InchiKey: KZJYHBWNCLVSOV-UHFFFAOYSA-N

Formula: C18H23F3O4

SMILES: CCCCCCCOC(=O)CCC(=O)OCc1c(F)ccc(F)c1F

Mol. weight [g/mol]: 360.37

Physical Properties

Property code	Value	Unit	Source
gf	-868.07	kJ/mol	Joback Method
hf	-1290.66	kJ/mol	Joback Method
hfus	50.06	kJ/mol	Joback Method
hvap	75.78	kJ/mol	Joback Method
log10ws	-5.68		Crippen Method
logp	4.441		Crippen Method
mcvol	260.910	ml/mol	McGowan Method
pc	1368.70	kPa	Joback Method
rinpol	2219.00		NIST Webbook
rinpol	2219.00		NIST Webbook
tb	803.25	K	Joback Method
tc	991.53	K	Joback Method
tf	502.69	K	Joback Method
vc	1.038	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	782.37	J/mol×K	803.25	Joback Method
cpg	796.60	J/mol×K	834.63	Joback Method
cpg	809.91	J/mol×K	866.01	Joback Method
cpg	822.31	J/mol×K	897.39	Joback Method
cpg	833.80	J/mol×K	928.77	Joback Method
cpg	844.39	J/mol×K	960.15	Joback Method
cpg	854.10	J/mol×K	991.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381179&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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