Succinic acid, hexyl 4-trifluoromethylbenzyl ester

Inchi: InChI=1S/C18H23F3O4/c1-2-3-4-5-12-24-16(22)10-11-17(23)25-13-14-6-8-15(9-7-14)18

InchiKey: MALRVBAKCNKPSW-UHFFFAOYSA-N

Formula: C18H23F3O4

SMILES: CCCCCCOC(=O)CCC(=O)OCc1ccc(C(F)(F)F)cc1

Mol. weight [g/mol]: 360.37

Physical Properties

Property code	Value	Unit	Source
gf	-845.97	kJ/mol	Joback Method
hf	-1276.47	kJ/mol	Joback Method
hfus	43.43	kJ/mol	Joback Method
hvap	73.17	kJ/mol	Joback Method
log10ws	-5.37		Crippen Method
logp	4.652		Crippen Method
mcvol	260.910	ml/mol	McGowan Method
pc	1419.71	kPa	Joback Method
rinpol	2112.00		NIST Webbook
rinpol	2112.00		NIST Webbook
tb	790.06	K	Joback Method
tc	980.80	K	Joback Method
tf	480.07	K	Joback Method
vc	1.026	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	785.53	J/mol×K	790.06	Joback Method
cpg	799.99	J/mol×K	821.85	Joback Method
cpg	813.48	J/mol×K	853.64	Joback Method
cpg	826.05	J/mol×K	885.43	Joback Method
cpg	837.71	J/mol×K	917.22	Joback Method
cpg	848.52	J/mol×K	949.01	Joback Method
cpg	858.49	J/mol×K	980.80	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382444&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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