Succinic acid, isobutyl 4-trifluoromethoxybenzyl ester

Inchi: InChI=1S/C16H19F3O5/c1-11(2)9-22-14(20)7-8-15(21)23-10-12-3-5-13(6-4-12)24-16(17

InchiKey: NMYJFJVMHQIMRX-UHFFFAOYSA-N

Formula: C16H19F3O5

SMILES: CC(C)COC(=O)CCC(=O)OCc1ccc(OC(F)(F)F)cc1

Mol. weight [g/mol]: 348.31

Physical Properties

Property code	Value	Unit	Source
gf	-970.25	kJ/mol	Joback Method
hf	-1372.69	kJ/mol	Joback Method
hfus	35.91	kJ/mol	Joback Method
hvap	70.73	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	3.608		Crippen Method
mcvol	238.600	ml/mol	McGowan Method
pc	1637.78	kPa	Joback Method
rinpol	1873.00		NIST Webbook
rinpol	1873.00		NIST Webbook
tb	766.28	K	Joback Method
tc	959.39	K	Joback Method
tf	464.76	K	Joback Method
vc	0.926	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	701.82	J/mol×K	766.28	Joback Method
cpg	715.47	J/mol×K	798.46	Joback Method
cpg	728.17	J/mol×K	830.65	Joback Method
cpg	739.93	J/mol×K	862.83	Joback Method
cpg	750.77	J/mol×K	895.02	Joback Method
cpg	760.72	J/mol×K	927.20	Joback Method
cpg	769.78	J/mol×K	959.39	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=U381561&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