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

Inchi: InChI=1S/C16H19F3O4/c1-2-3-4-9-22-14(20)7-8-15(21)23-10-11-12(17)5-6-13(18)16(11

InchiKey: IXROQNPATLUFHC-UHFFFAOYSA-N

Formula: C16H19F3O4

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

Mol. weight [g/mol]: 332.31

Physical Properties

Property code	Value	Unit	Source
gf	-884.91	kJ/mol	Joback Method
hf	-1249.38	kJ/mol	Joback Method
hfus	44.88	kJ/mol	Joback Method
hvap	71.33	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	3.661		Crippen Method
mcvol	232.730	ml/mol	McGowan Method
pc	1586.01	kPa	Joback Method
rinpol	2020.00		NIST Webbook
rinpol	2020.00		NIST Webbook
tb	757.49	K	Joback Method
tc	943.91	K	Joback Method
tf	480.15	K	Joback Method
vc	0.925	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	669.92	J/mol×K	757.49	Joback Method
cpg	683.36	J/mol×K	788.56	Joback Method
cpg	695.99	J/mol×K	819.63	Joback Method
cpg	707.80	J/mol×K	850.70	Joback Method
cpg	718.81	J/mol×K	881.77	Joback Method
cpg	729.02	J/mol×K	912.84	Joback Method
cpg	738.42	J/mol×K	943.91	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381176&Units=SI

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