Succinic acid, dodecyl 2-(trifluoromethyl)benzyl ester

Inchi: InChI=1S/C24H35F3O4/c1-2-3-4-5-6-7-8-9-10-13-18-30-22(28)16-17-23(29)31-19-20-14

InchiKey: CEJYBXRUDHZRAM-UHFFFAOYSA-N

Formula: C24H35F3O4

SMILES: CCCCCCCCCCCCOC(=O)CCC(=O)OCc1ccccc1C(F)(F)F

Mol. weight [g/mol]: 444.53

Physical Properties

Property code	Value	Unit	Source
gf	-795.45	kJ/mol	Joback Method
hf	-1400.31	kJ/mol	Joback Method
hfus	58.97	kJ/mol	Joback Method
hvap	86.52	kJ/mol	Joback Method
log10ws	-7.88		Crippen Method
logp	6.993		Crippen Method
mcvol	345.450	ml/mol	McGowan Method
pc	958.51	kPa	Joback Method
rinpol	2716.00		NIST Webbook
rinpol	2716.00		NIST Webbook
tb	927.34	K	Joback Method
tc	1135.40	K	Joback Method
tf	547.69	K	Joback Method
vc	1.363	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1140.63	J/mol×K	927.34	Joback Method
cpg	1157.09	J/mol×K	962.02	Joback Method
cpg	1172.28	J/mol×K	996.69	Joback Method
cpg	1186.27	J/mol×K	1031.37	Joback Method
cpg	1199.10	J/mol×K	1066.04	Joback Method
cpg	1210.85	J/mol×K	1100.72	Joback Method
cpg	1221.57	J/mol×K	1135.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381661&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

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