Succinic acid, hexadecyl 2-(trifluoromethyl)benzyl ester

Inchi: InChI=1S/C28H43F3O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-17-22-34-26(32)20-21-27(33

InchiKey: MJHAMEOSXXTYKK-UHFFFAOYSA-N

Formula: C28H43F3O4

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

Mol. weight [g/mol]: 500.63

Physical Properties

Property code	Value	Unit	Source
gf	-761.77	kJ/mol	Joback Method
hf	-1482.87	kJ/mol	Joback Method
hfus	69.33	kJ/mol	Joback Method
hvap	95.42	kJ/mol	Joback Method
log10ws	-9.55		Crippen Method
logp	8.553		Crippen Method
mcvol	401.810	ml/mol	McGowan Method
pc	765.64	kPa	Joback Method
rinpol	3115.00		NIST Webbook
rinpol	3115.00		NIST Webbook
tb	1018.86	K	Joback Method
tc	1257.93	K	Joback Method
tf	592.77	K	Joback Method
vc	1.587	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1389.35	J/mol×K	1018.86	Joback Method
cpg	1407.74	J/mol×K	1058.70	Joback Method
cpg	1424.47	J/mol×K	1098.55	Joback Method
cpg	1439.64	J/mol×K	1138.39	Joback Method
cpg	1453.36	J/mol×K	1178.24	Joback Method
cpg	1465.74	J/mol×K	1218.08	Joback Method
cpg	1476.88	J/mol×K	1257.93	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381665&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

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