Succinic acid, pentadecyl 2-(trifluoromethyl)benzyl ester

Inchi: InChI=1S/C27H41F3O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-21-33-25(31)19-20-26(32)34
InchiKey: RHNMJKCJKLYXTD-UHFFFAOYSA-N
Formula: C27H41F3O4
SMILES: CCCCCCCCCCCCCCCOC(=O)CCC(=O)OCc1ccccc1C(F)(F)F
Mol. weight [g/mol]: 486.61

Physical Properties

Property code	Value	Unit	Source
gf	-770.19	kJ/mol	Joback Method
hf	-1462.23	kJ/mol	Joback Method
hfus	66.74	kJ/mol	Joback Method
hvap	93.20	kJ/mol	Joback Method
log10ws	-9.13		Crippen Method
logp	8.163		Crippen Method
mcvol	387.720	ml/mol	McGowan Method
pc	807.99	kPa	Joback Method
tb	995.98	K	Joback Method
tc	1225.49	K	Joback Method
tf	581.50	K	Joback Method
vc	1.530	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1326.49	J/mol×K	995.98	Joback Method
cpg	1344.33	J/mol×K	1034.23	Joback Method
cpg	1360.62	J/mol×K	1072.48	Joback Method
cpg	1375.46	J/mol×K	1110.73	Joback Method
cpg	1388.94	J/mol×K	1148.98	Joback Method
cpg	1401.15	J/mol×K	1187.23	Joback Method
cpg	1412.18	J/mol×K	1225.49	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=U381664&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume