Succinic acid, tetradecyl 2,4,5-trifluorobenzyl ester

Inchi: InChI=1S/C25H37F3O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-31-24(29)14-15-25(30)32-19

InchiKey: HLEZWCANHRWTOL-UHFFFAOYSA-N

Formula: C25H37F3O4

SMILES: CCCCCCCCCCCCCCOC(=O)CCC(=O)OCc1cc(F)c(F)cc1F

Mol. weight [g/mol]: 458.55

Physical Properties

Property code	Value	Unit	Source
gf	-809.13	kJ/mol	Joback Method
hf	-1435.14	kJ/mol	Joback Method
hfus	68.19	kJ/mol	Joback Method
hvap	91.37	kJ/mol	Joback Method
log10ws	-8.61		Crippen Method
logp	7.172		Crippen Method
mcvol	359.540	ml/mol	McGowan Method
pc	877.91	kPa	Joback Method
rinpol	2865.00		NIST Webbook
rinpol	2865.00		NIST Webbook
tb	963.41	K	Joback Method
tc	1183.18	K	Joback Method
tf	581.58	K	Joback Method
vc	1.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1200.79	J/mol×K	963.41	Joback Method
cpg	1217.72	J/mol×K	1000.04	Joback Method
cpg	1233.10	J/mol×K	1036.67	Joback Method
cpg	1246.97	J/mol×K	1073.29	Joback Method
cpg	1259.36	J/mol×K	1109.92	Joback Method
cpg	1270.32	J/mol×K	1146.55	Joback Method
cpg	1279.87	J/mol×K	1183.18	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=U382229&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

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