

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

Inchi:	InChI=1S/C25H37F3O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-18-31-23(29)16-17-24(30)32-19
InchiKey:	KTDQQLLPQZJAQV-UHFFFAOYSA-N
Formula:	C25H37F3O4
SMILES:	CCCCCCCCCCCCCOC(=O)CCC(=O)OCc1c(F)ccc(F)c1F
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
mvol	359.540	ml/mol	McGowan Method
pc	877.91	kPa	Joback Method
rinpol	2915.00		NIST Webbook
rinpol	2915.00		NIST Webbook
tb	963.41	K	Joback Method
tc	1183.18	K	Joback Method
tf	581.58	K	Joback Method
vc	1.429	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U381185&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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