

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

Inchi:	InChI=1S/C24H35F3O4/c1-2-3-4-5-6-7-8-9-10-11-12-17-30-22(28)15-16-23(29)31-18-19
InchiKey:	PQVRUVZZAJVFSK-UHFFFAOYSA-N
Formula:	C24H35F3O4
SMILES:	CCCCCCCCCCCCOC(=O)CCC(=O)OCc1c(F)ccc(F)c1F
Mol. weight [g/mol]:	444.53

Physical Properties

Property code	Value	Unit	Source
gf	-817.55	kJ/mol	Joback Method
hf	-1414.50	kJ/mol	Joback Method
hfus	65.60	kJ/mol	Joback Method
hvap	89.14	kJ/mol	Joback Method
log10ws	-8.19		Crippen Method
logp	6.782		Crippen Method
mvol	345.450	ml/mol	McGowan Method
pc	930.07	kPa	Joback Method
rinpol	2818.00		NIST Webbook
rinpol	2818.00		NIST Webbook
tb	940.53	K	Joback Method
tc	1152.88	K	Joback Method
tf	570.31	K	Joback Method
vc	1.373	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1139.20	J/molxK	940.53	Joback Method
cpg	1155.70	J/molxK	975.92	Joback Method
cpg	1170.78	J/molxK	1011.31	Joback Method
cpg	1184.48	J/molxK	1046.71	Joback Method
cpg	1196.81	J/molxK	1082.10	Joback Method
cpg	1207.82	J/molxK	1117.49	Joback Method
cpg	1217.53	J/molxK	1152.88	Joback Method

Sources

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=U381184&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/114-385-8/Succinic-acid-tridecyl-2-3-6-trifluorobenzyl-ester.pdf>

Generated by Cheméo on 2024-05-04 16:35:34.540101577 +0000 UTC m=+17129783.460678899.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.