

Succinic acid, 3,4-difluorobenzyl tetradecyl ester

Inchi:	InChI=1S/C25H38F2O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-18-30-24(28)16-17-25(29)31-20
InchiKey:	QWDIVBXFWXNWHV-UHFFFAOYSA-N
Formula:	C25H38F2O4
SMILES:	CCCCCCCCCCCCCOC(=O)CCC(=O)OCc1ccc(F)c(F)c1
Mol. weight [g/mol]:	440.56

Physical Properties

Property code	Value	Unit	Source
gf	-604.69	kJ/mol	Joback Method
hf	-1227.56	kJ/mol	Joback Method
hfus	65.50	kJ/mol	Joback Method
hvap	91.52	kJ/mol	Joback Method
log10ws	-8.27		Crippen Method
logp	7.032		Crippen Method
mvol	357.770	ml/mol	McGowan Method
pc	909.98	kPa	Joback Method
rinpol	2928.00		NIST Webbook
rinpol	2928.00		NIST Webbook
tb	959.16	K	Joback Method
tc	1175.88	K	Joback Method
tf	568.47	K	Joback Method
vc	1.411	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1194.53	J/molxK	959.16	Joback Method
cpg	1211.56	J/molxK	995.28	Joback Method
cpg	1227.10	J/molxK	1031.40	Joback Method
cpg	1241.18	J/molxK	1067.52	Joback Method
cpg	1253.86	J/molxK	1103.64	Joback Method
cpg	1265.16	J/molxK	1139.76	Joback Method
cpg	1275.14	J/molxK	1175.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381752&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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