

Succinic acid, 2-chloro-6-fluorobenzyl pentadecyl ester

Inchi:	InChI=1S/C26H40ClFO4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-20-31-25(29)18-19-26(30)3
InchiKey:	LVDJQWJKZGEZJZ-UHFFFAOYSA-N
Formula:	C26H40ClFO4
SMILES:	CCCCCCCCCCCCCOC(=O)CCC(=O)OCc1c(F)cccc1Cl
Mol. weight [g/mol]:	471.05

Physical Properties

Property code	Value	Unit	Source
gf	-413.39	kJ/mol	Joback Method
hf	-1067.83	kJ/mol	Joback Method
hfus	69.21	kJ/mol	Joback Method
hvap	98.95	kJ/mol	Joback Method
log10ws	-9.05		Crippen Method
logp	7.937		Crippen Method
mcvol	382.330	ml/mol	McGowan Method
pc	863.53	kPa	Joback Method
tb	1020.20	K	Joback Method
tc	1253.10	K	Joback Method
tf	609.07	K	Joback Method
vc	1.498	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1275.61	J/molxK	1020.20	Joback Method
cpg	1291.87	J/molxK	1059.02	Joback Method
cpg	1306.47	J/molxK	1097.83	Joback Method
cpg	1319.45	J/molxK	1136.65	Joback Method
cpg	1330.87	J/molxK	1175.46	Joback Method
cpg	1340.79	J/molxK	1214.28	Joback Method
cpg	1349.27	J/molxK	1253.10	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=U380871&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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