Succinic acid, 4-fluorobenzyl heptadecyl ester

Inchi: InChI=1S/C28H45FO4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-23-32-27(30)21-22-28(
InchiKey: MSVIPPQDBAEGLX-UHFFFAOYSA-N
Formula: C28H45FO4
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)CCC(=O)OCc1ccc(F)cc1
Mol. weight [g/mol]: 464.65

Physical Properties

Property code	Value	Unit	Source
hf	-1182.11	kJ/mol	Cheméo Relay (1.0)
hfus	73.75	kJ/mol	Joback Method
hvap	136.06	kJ/mol	Cheméo Relay (1.0)
ie	9.06	eV	Cheméo Relay (1.0)
log10ws	-7.94		Cheméo Relay (1.0)
logp	8.064		Crippen Method
mcvol	398.270	ml/mol	McGowan Method
pc	761.00	kPa	Joback Method
rinpol	3234.00		NIST Webbook
rinpol	3234.00		NIST Webbook
tb	690.92	K	Cheméo Relay (1.0)
tc	881.21	K	Cheméo Relay (1.0)
tf	309.08	K	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	1.47390e+01
Coeff. B	2.42762e+00
Coeff. C	-1.29076e-03
Coeff. D	2.14000e-07
Coeff. E	0.00000e+00
Basis	predicted

Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381683&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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

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