Succinic acid, 2,2,3,3,4,4,4-heptafluorobutyl tetradecyl ester

Inchi: InChI=1S/C22H35F7O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-32-18(30)14-15-19(31)33-17

InchiKey: FOVKHQQJGXUGIO-UHFFFAOYSA-N

Formula: C22H35F7O4

SMILES: CCCCCCCCCCCCCCOC(=O)CCC(=O)OCC(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 496.50

Physical Properties

Property code	Value	Unit	Source
gf	-1688.63	kJ/mol	Joback Method
hf	-2386.03	kJ/mol	Joback Method
hfus	57.63	kJ/mol	Joback Method
hvap	73.27	kJ/mol	Joback Method
log10ws	-8.05		Crippen Method
logp	7.387		Crippen Method
mcvol	348.110	ml/mol	McGowan Method
pc	818.20	kPa	Joback Method
rinpol	2242.00		NIST Webbook
rinpol	2242.00		NIST Webbook
tb	840.54	K	Joback Method
tc	1031.22	K	Joback Method
tf	493.41	K	Joback Method
vc	1.409	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1144.76	J/mol×K	840.54	Joback Method
cpg	1162.51	J/mol×K	872.32	Joback Method
cpg	1179.14	J/mol×K	904.10	Joback Method
cpg	1194.72	J/mol×K	935.88	Joback Method
cpg	1209.33	J/mol×K	967.66	Joback Method
cpg	1223.03	J/mol×K	999.44	Joback Method
cpg	1235.91	J/mol×K	1031.22	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U382361&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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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