Succinic acid, 2,2,3,3,4,4,5,5-octafluoropentyl neopentyl ester

Inchi: InChI=1S/C14H18F8O4/c1-11(2,3)6-25-8(23)4-5-9(24)26-7-12(17,18)14(21,22)13(19,20)

InchiKey: WYEDCKOWPWMKNR-UHFFFAOYSA-N

Formula: C14H18F8O4

SMILES: CC(C)(C)COC(=O)CCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 402.28

Physical Properties

Property code	Value	Unit	Source
gf	-1950.40	kJ/mol	Joback Method
hf	-2431.05	kJ/mol	Joback Method
hfus	29.05	kJ/mol	Joback Method
hvap	52.96	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	4.070		Crippen Method
mcvol	237.160	ml/mol	McGowan Method
pc	1326.17	kPa	Joback Method
rinpol	1460.00		NIST Webbook
rinpol	1460.00		NIST Webbook
tb	653.10	K	Joback Method
tc	814.67	K	Joback Method
tf	391.26	K	Joback Method
vc	0.962	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	696.88	J/mol×K	653.10	Joback Method
cpg	710.38	J/mol×K	680.03	Joback Method
cpg	723.05	J/mol×K	706.96	Joback Method
cpg	734.95	J/mol×K	733.88	Joback Method
cpg	746.11	J/mol×K	760.81	Joback Method
cpg	756.58	J/mol×K	787.74	Joback Method
cpg	766.39	J/mol×K	814.67	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=U389576&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