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

Inchi: InChI=1S/C20H31F7O4/c1-2-3-4-5-6-7-8-9-10-11-14-30-16(28)12-13-17(29)31-15-18(21

InchiKey: PAKDXCUVQKNEGK-UHFFFAOYSA-N

Formula: C20H31F7O4

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

Mol. weight [g/mol]: 468.45

Physical Properties

Property code	Value	Unit	Source
gf	-1705.47	kJ/mol	Joback Method
hf	-2344.75	kJ/mol	Joback Method
hfus	52.45	kJ/mol	Joback Method
hvap	68.82	kJ/mol	Joback Method
log10ws	-7.21		Crippen Method
logp	6.607		Crippen Method
mcvol	319.930	ml/mol	McGowan Method
pc	916.05	kPa	Joback Method
rinpol	2051.00		NIST Webbook
rinpol	2051.00		NIST Webbook
tb	794.78	K	Joback Method
tc	973.05	K	Joback Method
tf	470.87	K	Joback Method
vc	1.296	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1024.67	J/mol×K	794.78	Joback Method
cpg	1041.13	J/mol×K	824.49	Joback Method
cpg	1056.61	J/mol×K	854.20	Joback Method
cpg	1071.15	J/mol×K	883.91	Joback Method
cpg	1084.81	J/mol×K	913.63	Joback Method
cpg	1097.66	J/mol×K	943.34	Joback Method
cpg	1109.74	J/mol×K	973.05	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=U382359&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