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

Inchi: InChI=1S/C28H47F7O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-22-38-24(36
InchiKey: REHPFPKNOBXOQJ-UHFFFAOYSA-N
Formula: C28H47F7O4
SMILES: CCCCCCCCCCCCCCCCCCCCCOC(=O)CCC(=O)OCC(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 580.66

Physical Properties

Property code	Value	Unit	Source
gf	-1638.11	kJ/mol	Joback Method
hf	-2509.87	kJ/mol	Joback Method
hfus	73.17	kJ/mol	Joback Method
hvap	86.63	kJ/mol	Joback Method
log10ws	-10.56		Crippen Method
logp	9.728		Crippen Method
mcvol	432.650	ml/mol	McGowan Method
pc	603.09	kPa	Joback Method
rinpol	2805.00		NIST Webbook
rinpol	2805.00		NIST Webbook
tb	977.82	K	Joback Method
tc	1233.31	K	Joback Method
tf	561.03	K	Joback Method
vc	1.744	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1520.38	J/mol×K	977.82	Joback Method
cpg	1543.79	J/mol×K	1020.40	Joback Method
cpg	1565.41	J/mol×K	1062.98	Joback Method
cpg	1585.44	J/mol×K	1105.56	Joback Method
cpg	1604.09	J/mol×K	1148.15	Joback Method
cpg	1621.57	J/mol×K	1190.73	Joback Method
cpg	1638.09	J/mol×K	1233.31	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=U382366&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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