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

Inchi: InChI=1S/C15H9F11O4/c16-6-1-2-7(11(18)10(6)17)30-9(28)4-3-8(27)29-5-13(21,22)15(2

InchiKey: USXNPOQGHKICSS-UHFFFAOYSA-N

Formula: C15H9F11O4

SMILES: O=C(CCC(=O)Oc1ccc(F)c(F)c1F)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 462.21

Physical Properties

Property code	Value	Unit	Source
gf	-2445.73	kJ/mol	Joback Method
hf	-2829.15	kJ/mol	Joback Method
hfus	41.17	kJ/mol	Joback Method
hvap	58.30	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	4.504		Crippen Method
mcvol	232.800	ml/mol	McGowan Method
pc	1361.64	kPa	Joback Method
rinpol	1708.00		NIST Webbook
tb	718.64	K	Joback Method
tc	887.48	K	Joback Method
tf	465.86	K	Joback Method
vc	0.975	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	686.11	J/mol×K	718.64	Joback Method
cpg	696.70	J/mol×K	746.78	Joback Method
cpg	706.56	J/mol×K	774.92	Joback Method
cpg	715.72	J/mol×K	803.06	Joback Method
cpg	724.22	J/mol×K	831.20	Joback Method
cpg	732.09	J/mol×K	859.34	Joback Method
cpg	739.38	J/mol×K	887.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390755&Units=SI
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

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