Succinic acid, 2,2,3,3,4,4,5,5-octafluoropentyl 2-fluoro-3-(trifluoromethyl)phenyl ester

Inchi: InChI=1S/C16H10F12O4/c17-11-7(15(24,25)26)2-1-3-8(11)32-10(30)5-4-9(29)31-6-13(2

InchiKey: NDDYNDOIFACPLU-UHFFFAOYSA-N

Formula: C16H10F12O4

SMILES: O=C(CCC(=O)Oc1cccc(C(F)(F)F)c1F)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 494.23

Physical Properties

Property code	Value	Unit	Source
gf	-2619.65	kJ/mol	Joback Method
hf	-3043.18	kJ/mol	Joback Method
hfus	39.81	kJ/mol	Joback Method
hvap	57.75	kJ/mol	Joback Method
log10ws	-6.27		Crippen Method
logp	5.244		Crippen Method
mcvol	248.660	ml/mol	McGowan Method
pc	1260.16	kPa	Joback Method
rinpol	1721.00		NIST Webbook
rinpol	1721.00		NIST Webbook
tb	732.58	K	Joback Method
tc	902.66	K	Joback Method
tf	467.62	K	Joback Method
vc	1.038	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	750.61	J/mol×K	732.58	Joback Method
cpg	761.50	J/mol×K	760.93	Joback Method
cpg	771.58	J/mol×K	789.27	Joback Method
cpg	780.91	J/mol×K	817.62	Joback Method
cpg	789.55	J/mol×K	845.97	Joback Method
cpg	797.53	J/mol×K	874.31	Joback Method
cpg	804.92	J/mol×K	902.66	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=U390778&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