Succinic acid, 2,2,3,3-tetrafluoropropyl 2-fluoro-3-(trifluoromethyl)phenyl ester

Inchi: InChI=1S/C14H10F8O4/c15-11-7(14(20,21)22)2-1-3-8(11)26-10(24)5-4-9(23)25-6-13(18

InchiKey: PXIAKFLSSUVBGK-UHFFFAOYSA-N

Formula: C14H10F8O4

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

Mol. weight [g/mol]: 394.21

Physical Properties

Property code	Value	Unit	Source
gf	-1862.93	kJ/mol	Joback Method
hf	-2199.96	kJ/mol	Joback Method
hfus	37.14	kJ/mol	Joback Method
hvap	59.15	kJ/mol	Joback Method
log10ws	-4.80		Crippen Method
logp	3.974		Crippen Method
mcvol	213.400	ml/mol	McGowan Method
pc	1621.98	kPa	Joback Method
rinpol	1644.00		NIST Webbook
rinpol	1644.00		NIST Webbook
tb	696.20	K	Joback Method
tc	870.38	K	Joback Method
tf	437.88	K	Joback Method
vc	0.875	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	608.42	J/mol×K	696.20	Joback Method
cpg	619.53	J/mol×K	725.23	Joback Method
cpg	629.89	J/mol×K	754.26	Joback Method
cpg	639.55	J/mol×K	783.29	Joback Method
cpg	648.53	J/mol×K	812.32	Joback Method
cpg	656.85	J/mol×K	841.35	Joback Method
cpg	664.56	J/mol×K	870.38	Joback Method

Sources

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=U390777&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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