

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

Inchi: InChI=1S/C15H13F7O4/c1-9-4-2-3-5-10(9)26-12(24)7-6-11(23)25-8-13(16,17)14(18,19)1
InchiKey: AOYVMAJVDCTSQM-UHFFFAOYSA-N
Formula: C15H13F7O4
SMILES: Cc1ccccc1OC(=O)CCC(=O)OCC(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 390.25

Physical Properties

Property code	Value	Unit	Source
gf	-1644.79	kJ/mol	Joback Method
hf	-2016.49	kJ/mol	Joback Method
hfus	33.15	kJ/mol	Joback Method
hvap	60.63	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	4.057		Crippen Method
mcvol	225.720	ml/mol	McGowan Method
pc	1589.81	kPa	Joback Method
rinsol	1676.00		NIST Webbook
tb	712.04	K	Joback Method
tc	894.09	K	Joback Method
tf	453.46	K	Joback Method
vc	0.908	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	656.14	J/molxK	712.04	Joback Method
cpg	668.19	J/molxK	742.38	Joback Method
cpg	679.37	J/molxK	772.72	Joback Method
cpg	689.73	J/molxK	803.06	Joback Method
cpg	699.33	J/molxK	833.41	Joback Method
cpg	708.21	J/molxK	863.75	Joback Method
cpg	716.42	J/molxK	894.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357531&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	McGowan's characteristic volume
pc:	Critical Pressure
r inpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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