

Succinic acid, 2,2,3,3-tetrafluoropropyl phenethyl ester

Inchi:	InChI=1S/C15H16F4O4/c16-14(17)15(18,19)10-23-13(21)7-6-12(20)22-9-8-11-4-2-1-3-5
InchiKey:	HRGYAARKGZHHHO-UHFFFAOYSA-N
Formula:	C15H16F4O4
SMILES:	O=C(CCC(=O)OCC(F)(F)C(F)F)OCCc1ccccc1
Mol. weight [g/mol]:	336.28

Physical Properties

Property code	Value	Unit	Source
gf	-1058.85	kJ/mol	Joback Method
hf	-1404.47	kJ/mol	Joback Method
hfus	35.60	kJ/mol	Joback Method
hvap	64.62	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	2.996		Crippen Method
mcvol	220.410	ml/mol	McGowan Method
pc	1753.60	kPa	Joback Method
rinpol	1843.00		NIST Webbook
rinpol	1843.00		NIST Webbook
tb	715.27	K	Joback Method
tc	902.44	K	Joback Method
tf	419.33	K	Joback Method
vc	0.871	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	628.83	J/molxK	715.27	Joback Method
cpg	642.09	J/molxK	746.47	Joback Method
cpg	654.47	J/molxK	777.66	Joback Method
cpg	666.01	J/molxK	808.86	Joback Method
cpg	676.73	J/molxK	840.05	Joback Method
cpg	686.67	J/molxK	871.25	Joback Method
cpg	695.85	J/molxK	902.44	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389741&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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