

Succinic acid, cyclohexylmethyl 2,2,3,4,4,4-hexafluorobutyl ester

Inchi:	InChI=1S/C15H20F6O4/c16-13(15(19,20)21)14(17,18)9-25-12(23)7-6-11(22)24-8-10-4-2
InchiKey:	OTUYIPXBCIRSHF-UHFFFAOYSA-N
Formula:	C15H20F6O4
SMILES:	O=C(CCC(=O)OCC(F)(F)C(F)C(F)(F)F)OCC1CCCCC1
Mol. weight [g/mol]:	378.31

Physical Properties

Property code	Value	Unit	Source
gf	-1533.59	kJ/mol	Joback Method
hf	-1987.65	kJ/mol	Joback Method
hfus	32.14	kJ/mol	Joback Method
hvap	59.84	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	3.969		Crippen Method
mcvol	236.850	ml/mol	McGowan Method
pc	1496.51	kPa	Joback Method
rinpol	1726.00		NIST Webbook
tb	703.45	K	Joback Method
tc	881.99	K	Joback Method
tf	403.89	K	Joback Method
vc	0.936	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	723.57	J/molxK	703.45	Joback Method
cpg	739.21	J/molxK	733.21	Joback Method
cpg	753.85	J/molxK	762.96	Joback Method
cpg	767.53	J/molxK	792.72	Joback Method
cpg	780.29	J/molxK	822.48	Joback Method
cpg	792.16	J/molxK	852.24	Joback Method
cpg	803.19	J/molxK	881.99	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390806&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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