

Succinic acid, 2,2,3,3,4,4,5,5-octafluoropentyl 2,2-dichloroethyl ester

Inchi:	InChI=1S/C11H10Cl2F8O4/c12-5(13)3-24-6(22)1-2-7(23)25-4-9(16,17)11(20,21)10(18,19)
InchiKey:	ZYOLSNDZRWZTLJ-UHFFFAOYSA-N
Formula:	C11H10Cl2F8O4
SMILES:	O=C(CCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F)OCC(Cl)Cl
Mol. weight [g/mol]:	429.09

Physical Properties

Property code	Value	Unit	Source
gf	-2004.80	kJ/mol	Joback Method
hf	-2397.14	kJ/mol	Joback Method
hfus	33.57	kJ/mol	Joback Method
hvap	55.96	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	3.828		Crippen Method
mcvol	219.370	ml/mol	McGowan Method
pc	1546.35	kPa	Joback Method
rinsol	1609.00		NIST Webbook
tb	662.11	K	Joback Method
tc	829.00	K	Joback Method
tf	399.87	K	Joback Method
vc	0.896	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	595.08	J/mol×K	662.11	Joback Method
cpg	605.35	J/mol×K	689.92	Joback Method
cpg	614.91	J/mol×K	717.74	Joback Method
cpg	623.81	J/mol×K	745.55	Joback Method
cpg	632.08	J/mol×K	773.37	Joback Method
cpg	639.76	J/mol×K	801.18	Joback Method
cpg	646.88	J/mol×K	829.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390515&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
mccvol:	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

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