

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

Inchi:	InChI=1S/C17H24F4O4/c1-12(2)5-4-6-13(3)9-10-24-14(22)7-8-15(23)25-11-17(20,21)16
InchiKey:	VTUSQBHLOIBRIV-LCYFTJDESA-N
Formula:	C17H24F4O4
SMILES:	CC(C)=CCCC(C)=CCOC(=O)CCC(=O)OCC(F)(F)C(F)F
Mol. weight [g/mol]:	368.36

Physical Properties

Property code	Value	Unit	Source
gf	-1011.08	kJ/mol	Joback Method
hf	-1467.42	kJ/mol	Joback Method
hfus	44.53	kJ/mol	Joback Method
hvap	66.87	kJ/mol	Joback Method
log10ws	-5.00		Crippen Method
logp	4.446		Crippen Method
mcvol	263.750	ml/mol	McGowan Method
pc	1278.25	kPa	Joback Method
rinpol	1892.00		NIST Webbook
rinpol	1892.00		NIST Webbook
tb	742.43	K	Joback Method
tc	920.32	K	Joback Method
tf	377.37	K	Joback Method
vc	1.052	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	775.88	J/mol×K	742.43	Joback Method
cpg	790.64	J/mol×K	772.08	Joback Method
cpg	804.60	J/mol×K	801.73	Joback Method
cpg	817.78	J/mol×K	831.38	Joback Method
cpg	830.23	J/mol×K	861.03	Joback Method
cpg	841.98	J/mol×K	890.67	Joback Method
cpg	853.08	J/mol×K	920.32	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=U391235&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

cp_g:	Ideal gas heat capacity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
pc:	Critical Pressure
rin_{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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