

Succinic acid, dec-2-yl 2-fluoroethyl ester

Inchi:	InChI=1S/C16H29FO4/c1-3-4-5-6-7-8-9-14(2)21-16(19)11-10-15(18)20-13-12-17/h14H,3
InchiKey:	ZNZUSRVBBJOKEQ-UHFFFAOYSA-N
Formula:	C16H29FO4
SMILES:	CCCCCCCCC(C)OC(=O)CCC(=O)OCCF
Mol. weight [g/mol]:	304.40

Physical Properties

Property code	Value	Unit	Source
gf	-581.25	kJ/mol	Joback Method
hf	-1064.56	kJ/mol	Joback Method
hfus	42.33	kJ/mol	Joback Method
hvap	68.32	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	3.962		Crippen Method
mcvol	252.950	ml/mol	McGowan Method
pc	1372.76	kPa	Joback Method
rinpol	1970.00		NIST Webbook
rinpol	1970.00		NIST Webbook
tb	716.89	K	Joback Method
tc	890.70	K	Joback Method
tf	399.99	K	Joback Method
vc	0.992	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	741.83	J/mol×K	716.89	Joback Method
cpg	758.12	J/mol×K	745.86	Joback Method
cpg	773.61	J/mol×K	774.83	Joback Method
cpg	788.30	J/mol×K	803.80	Joback Method
cpg	802.20	J/mol×K	832.76	Joback Method
cpg	815.32	J/mol×K	861.73	Joback Method
cpg	827.66	J/mol×K	890.70	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=U390884&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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