

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

Inchi:	InChI=1S/C17H31FO4/c1-3-4-5-6-7-8-10-15(2)22-17(20)12-9-11-16(19)21-14-13-18/h15
InchiKey:	CWDYWLXWXWAIBP-UHFFFAOYSA-N
Formula:	C17H31FO4
SMILES:	CCCCCCCC(C)OC(=O)CCCC(=O)OCCF
Mol. weight [g/mol]:	318.42

Physical Properties

Property code	Value	Unit	Source
gf	-572.83	kJ/mol	Joback Method
hf	-1085.20	kJ/mol	Joback Method
hfus	44.92	kJ/mol	Joback Method
hvap	70.54	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	4.352		Crippen Method
mvol	267.040	ml/mol	McGowan Method
pc	1280.08	kPa	Joback Method
rinpol	1989.00		NIST Webbook
rinpol	1989.00		NIST Webbook
tb	739.77	K	Joback Method
tc	914.84	K	Joback Method
tf	411.26	K	Joback Method
vc	1.048	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	799.18	J/mol×K	739.77	Joback Method
cpg	815.92	J/mol×K	768.95	Joback Method
cpg	831.80	J/mol×K	798.13	Joback Method
cpg	846.83	J/mol×K	827.30	Joback Method
cpg	861.03	J/mol×K	856.48	Joback Method
cpg	874.40	J/mol×K	885.66	Joback Method
cpg	886.95	J/mol×K	914.84	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=U393716&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.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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