Glutaric acid, dodec-2-en-1-yl 2-fluoroethyl ester

Inchi: InChI=1S/C19H33FO4/c1-2-3-4-5-6-7-8-9-10-11-16-23-18(21)13-12-14-19(22)24-17-15-2

InchiKey: OBOJRAXRNRJRGR-ZHACJKMWSA-N

Formula: C19H33FO4

SMILES: CCCCCCCCCC=CCOC(=O)CCCC(=O)OCCF

Mol. weight [g/mol]: 344.46

Physical Properties

Property code	Value	Unit	Source
gf	-473.33	kJ/mol	Joback Method
hf	-1003.98	kJ/mol	Joback Method
hfus	53.82	kJ/mol	Joback Method
hvap	75.34	kJ/mol	Joback Method
log10ws	-5.21		Crippen Method
logp	4.910		Crippen Method
mcvol	290.920	ml/mol	McGowan Method
pc	1154.57	kPa	Joback Method
rinpol	2299.00		NIST Webbook
rinpol	2299.00		NIST Webbook
tb	790.13	K	Joback Method
tc	971.24	K	Joback Method
tf	443.72	K	Joback Method
vc	1.145	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	891.59	J/mol×K	790.13	Joback Method
cpg	908.53	J/mol×K	820.32	Joback Method
cpg	924.54	J/mol×K	850.50	Joback Method
cpg	939.66	J/mol×K	880.69	Joback Method
cpg	953.91	J/mol×K	910.87	Joback Method
cpg	967.30	J/mol×K	941.06	Joback Method
cpg	979.86	J/mol×K	971.24	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393720&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume