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

Inchi: InChI=1S/C20H33F3O4/c1-3-4-5-6-7-8-9-10-11-12-16-26-18(24)14-13-15-19(25)27-17(2

InchiKey: HIMOKJZIQICGDT-VAWYXSNFSA-N

Formula: C20H33F3O4

SMILES: CCCCCCCCCC=CCOC(=O)CCCC(=O)OC(C)C(F)(F)F

Mol. weight [g/mol]: 394.47

Physical Properties

Property code	Value	Unit	Source
gf	-854.13	kJ/mol	Joback Method
hf	-1430.87	kJ/mol	Joback Method
hfus	51.63	kJ/mol	Joback Method
hvap	74.25	kJ/mol	Joback Method
log10ws	-6.55		Crippen Method
logp	5.891		Crippen Method
mcvol	308.550	ml/mol	McGowan Method
pc	1039.24	kPa	Joback Method
rinpol	2146.00		NIST Webbook
tb	807.88	K	Joback Method
tc	990.62	K	Joback Method
tf	443.59	K	Joback Method
vc	1.220	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	967.70	J/mol×K	807.88	Joback Method
cpg	984.57	J/mol×K	838.34	Joback Method
cpg	1000.47	J/mol×K	868.79	Joback Method
cpg	1015.43	J/mol×K	899.25	Joback Method
cpg	1029.51	J/mol×K	929.70	Joback Method
cpg	1042.74	J/mol×K	960.16	Joback Method
cpg	1055.15	J/mol×K	990.62	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393658&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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