Glutaric acid, dodec-2-en-1-yl 2,2,3,4,4,4-hexafluorobutyl ester

Inchi: InChI=1S/C21H32F6O4/c1-2-3-4-5-6-7-8-9-10-11-15-30-17(28)13-12-14-18(29)31-16-20

InchiKey: CDRLFMBPCUGTAH-ZHACJKMWSA-N

Formula: C21H32F6O4

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

Mol. weight [g/mol]: 462.47

Physical Properties

Property code	Value	Unit	Source
gf	-1427.30	kJ/mol	Joback Method
hf	-2048.59	kJ/mol	Joback Method
hfus	56.05	kJ/mol	Joback Method
hvap	72.73	kJ/mol	Joback Method
log10ws	-7.13		Crippen Method
logp	6.476		Crippen Method
mcvol	327.950	ml/mol	McGowan Method
pc	910.53	kPa	Joback Method
rinpol	2215.00		NIST Webbook
tb	825.34	K	Joback Method
tc	1010.55	K	Joback Method
tf	459.05	K	Joback Method
vc	1.319	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1050.78	J/mol×K	825.34	Joback Method
cpg	1067.50	J/mol×K	856.21	Joback Method
cpg	1083.21	J/mol×K	887.08	Joback Method
cpg	1097.98	J/mol×K	917.95	Joback Method
cpg	1111.86	J/mol×K	948.81	Joback Method
cpg	1124.92	J/mol×K	979.68	Joback Method
cpg	1137.21	J/mol×K	1010.55	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393697&Units=SI

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