Glutaric acid, dodec-2-en-1-yl 2,2,3,3,3-pentafluoropropyl ester

Inchi: InChI=1S/C20H31F5O4/c1-2-3-4-5-6-7-8-9-10-11-15-28-17(26)13-12-14-18(27)29-16-19

InchiKey: AXSRVOSRPCUWFW-ZHACJKMWSA-N

Formula: C20H31F5O4

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

Mol. weight [g/mol]: 430.45

Physical Properties

Property code	Value	Unit	Source
gf	-1238.47	kJ/mol	Joback Method
hf	-1826.56	kJ/mol	Joback Method
hfus	53.90	kJ/mol	Joback Method
hvap	71.71	kJ/mol	Joback Method
log10ws	-6.75		Crippen Method
logp	6.138		Crippen Method
mcvol	312.090	ml/mol	McGowan Method
pc	988.26	kPa	Joback Method
rinpol	2067.00		NIST Webbook
rinpol	2067.00		NIST Webbook
tb	803.63	K	Joback Method
tc	984.28	K	Joback Method
tf	462.19	K	Joback Method
vc	1.252	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	983.29	J/mol×K	803.63	Joback Method
cpg	999.56	J/mol×K	833.74	Joback Method
cpg	1014.88	J/mol×K	863.85	Joback Method
cpg	1029.33	J/mol×K	893.95	Joback Method
cpg	1042.93	J/mol×K	924.06	Joback Method
cpg	1055.76	J/mol×K	954.17	Joback Method
cpg	1067.85	J/mol×K	984.28	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393681&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