Glutaric acid, tridec-2-yn-1-yl 2,2,3,3,3-pentafluoropropyl ester

Inchi: InChI=1S/C21H31F5O4/c1-2-3-4-5-6-7-8-9-10-11-12-16-29-18(27)14-13-15-19(28)30-17

InchiKey: DZVRZHSMSUQVAY-UHFFFAOYSA-N

Formula: C21H31F5O4

SMILES: CCCCCCCCCCC#CCOC(=O)CCCC(=O)OCC(F)(F)C(F)(F)F

Mol. weight [g/mol]: 442.46

Physical Properties

Property code	Value	Unit	Source
gf	-1107.47	kJ/mol	Joback Method
hf	-1692.12	kJ/mol	Joback Method
hfus	59.41	kJ/mol	Joback Method
hvap	76.13	kJ/mol	Joback Method
log10ws	-7.11		Crippen Method
logp	5.975		Crippen Method
mcvol	321.880	ml/mol	McGowan Method
pc	995.76	kPa	Joback Method
rinpol	2189.00		NIST Webbook
tb	831.35	K	Joback Method
tc	1018.37	K	Joback Method
tf	584.64	K	Joback Method
vc	1.290	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1018.47	J/mol×K	831.35	Joback Method
cpg	1034.70	J/mol×K	862.52	Joback Method
cpg	1049.92	J/mol×K	893.69	Joback Method
cpg	1064.18	J/mol×K	924.86	Joback Method
cpg	1077.54	J/mol×K	956.03	Joback Method
cpg	1090.05	J/mol×K	987.20	Joback Method
cpg	1101.74	J/mol×K	1018.37	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=U393682&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