Glutaric acid, 1,1,1-trifluoroprop-2-yl pentadecyl ester

Inchi: InChI=1S/C23H41F3O4/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-19-29-21(27)17-16-18-22(2

InchiKey: XBPISTPHJJNWPX-UHFFFAOYSA-N

Formula: C23H41F3O4

SMILES: CCCCCCCCCCCCCCCOC(=O)CCCC(=O)OC(C)C(F)(F)F

Mol. weight [g/mol]: 438.56

Physical Properties

Property code	Value	Unit	Source
gf	-909.09	kJ/mol	Joback Method
hf	-1610.01	kJ/mol	Joback Method
hfus	59.20	kJ/mol	Joback Method
hvap	80.97	kJ/mol	Joback Method
log10ws	-7.95		Crippen Method
logp	7.285		Crippen Method
mcvol	355.120	ml/mol	McGowan Method
pc	844.07	kPa	Joback Method
rinpol	2454.00		NIST Webbook
rinpol	2454.00		NIST Webbook
tb	872.36	K	Joback Method
tc	1069.44	K	Joback Method
tf	482.48	K	Joback Method
vc	1.409	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1176.71	J/mol×K	872.36	Joback Method
cpg	1195.85	J/mol×K	905.21	Joback Method
cpg	1213.73	J/mol×K	938.05	Joback Method
cpg	1230.39	J/mol×K	970.90	Joback Method
cpg	1245.89	J/mol×K	1003.75	Joback Method
cpg	1260.25	J/mol×K	1036.59	Joback Method
cpg	1273.55	J/mol×K	1069.44	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=U391652&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