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

Inchi: InChI=1S/C26H47F3O4/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-22-32-24(30)20-1

InchiKey: VRSJXETWDULVLL-UHFFFAOYSA-N

Formula: C26H47F3O4

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

Mol. weight [g/mol]: 480.64

Physical Properties

Property code	Value	Unit	Source
gf	-883.83	kJ/mol	Joback Method
hf	-1671.93	kJ/mol	Joback Method
hfus	66.97	kJ/mol	Joback Method
hvap	87.65	kJ/mol	Joback Method
log10ws	-9.21		Crippen Method
logp	8.455		Crippen Method
mcvol	397.390	ml/mol	McGowan Method
pc	718.76	kPa	Joback Method
rinpol	2747.00		NIST Webbook
rinpol	2747.00		NIST Webbook
tb	941.00	K	Joback Method
tc	1163.51	K	Joback Method
tf	516.29	K	Joback Method
vc	1.577	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1365.97	J/mol×K	941.00	Joback Method
cpg	1387.19	J/mol×K	978.08	Joback Method
cpg	1406.77	J/mol×K	1015.17	Joback Method
cpg	1424.78	J/mol×K	1052.25	Joback Method
cpg	1441.32	J/mol×K	1089.34	Joback Method
cpg	1456.45	J/mol×K	1126.42	Joback Method
cpg	1470.26	J/mol×K	1163.51	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=U391641&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