Glutaric acid, 2,2,2-triluoroethyl eicosyl ester

Inchi: InChI=1S/C27H49F3O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-23-33-25(31
InchiKey: PBNINDCQRGMTPP-UHFFFAOYSA-N
Formula: C27H49F3O4
SMILES: CCCCCCCCCCCCCCCCCCCCOC(=O)CCCC(=O)OCC(F)(F)F
Mol. weight [g/mol]: 494.67

Physical Properties

Property code	Value	Unit	Source
gf	-872.97	kJ/mol	Joback Method
hf	-1687.29	kJ/mol	Joback Method
hfus	73.09	kJ/mol	Joback Method
hvap	90.26	kJ/mol	Joback Method
log10ws	-9.51		Crippen Method
logp	8.847		Crippen Method
mcvol	411.480	ml/mol	McGowan Method
pc	680.29	kPa	Joback Method
rinpol	2889.00		NIST Webbook
rinpol	2889.00		NIST Webbook
tb	964.32	K	Joback Method
tc	1200.34	K	Joback Method
tf	542.56	K	Joback Method
vc	1.639	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1429.69	J/mol×K	964.32	Joback Method
cpg	1452.00	J/mol×K	1003.66	Joback Method
cpg	1472.48	J/mol×K	1042.99	Joback Method
cpg	1491.23	J/mol×K	1082.33	Joback Method
cpg	1508.36	J/mol×K	1121.67	Joback Method
cpg	1523.95	J/mol×K	1161.00	Joback Method
cpg	1538.11	J/mol×K	1200.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380526&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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