Glutaric acid, 2,2,2-triluoroethyl octadecyl ester

Inchi: InChI=1S/C25H45F3O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-21-31-23(29)19-18

InchiKey: UASPBCMXJCKPLM-UHFFFAOYSA-N

Formula: C25H45F3O4

SMILES: CCCCCCCCCCCCCCCCCCOC(=O)CCCC(=O)OCC(F)(F)F

Mol. weight [g/mol]: 466.62

Physical Properties

Property code	Value	Unit	Source
gf	-889.81	kJ/mol	Joback Method
hf	-1646.01	kJ/mol	Joback Method
hfus	67.91	kJ/mol	Joback Method
hvap	85.81	kJ/mol	Joback Method
log10ws	-8.67		Crippen Method
logp	8.067		Crippen Method
mcvol	383.300	ml/mol	McGowan Method
pc	753.91	kPa	Joback Method
rinpol	2696.00		NIST Webbook
rinpol	2696.00		NIST Webbook
tb	918.56	K	Joback Method
tc	1133.04	K	Joback Method
tf	520.02	K	Joback Method
vc	1.526	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1301.96	J/mol×K	918.56	Joback Method
cpg	1322.61	J/mol×K	954.31	Joback Method
cpg	1341.75	J/mol×K	990.05	Joback Method
cpg	1359.46	J/mol×K	1025.80	Joback Method
cpg	1375.79	J/mol×K	1061.54	Joback Method
cpg	1390.82	J/mol×K	1097.29	Joback Method
cpg	1404.61	J/mol×K	1133.04	Joback Method

Sources

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=U380525&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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