Glutaric acid, 2,2,3,3-tetrafluoropropyl dodecyl ester

Inchi: InChI=1S/C20H34F4O4/c1-2-3-4-5-6-7-8-9-10-11-15-27-17(25)13-12-14-18(26)28-16-20

InchiKey: PORGMEVSQOIHDH-UHFFFAOYSA-N

Formula: C20H34F4O4

SMILES: CCCCCCCCCCCCOC(=O)CCCC(=O)OCC(F)(F)C(F)F

Mol. weight [g/mol]: 414.48

Physical Properties

Property code	Value	Unit	Source
gf	-1129.16	kJ/mol	Joback Method
hf	-1744.20	kJ/mol	Joback Method
hfus	54.51	kJ/mol	Joback Method
hvap	73.47	kJ/mol	Joback Method
log10ws	-6.55		Crippen Method
logp	6.064		Crippen Method
mcvol	314.620	ml/mol	McGowan Method
pc	977.17	kPa	Joback Method
rinpol	2224.00		NIST Webbook
rinpol	2224.00		NIST Webbook
tb	802.99	K	Joback Method
tc	983.16	K	Joback Method
tf	449.26	K	Joback Method
vc	1.258	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1000.39	J/mol×K	802.99	Joback Method
cpg	1017.73	J/mol×K	833.02	Joback Method
cpg	1034.05	J/mol×K	863.05	Joback Method
cpg	1049.39	J/mol×K	893.07	Joback Method
cpg	1063.77	J/mol×K	923.10	Joback Method
cpg	1077.23	J/mol×K	953.13	Joback Method
cpg	1089.80	J/mol×K	983.16	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=U391595&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