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

Inchi: InChI=1S/C23H40F4O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-18-30-20(28)16-15-17-21(29

InchiKey: SGUNCYBPPFKOPS-UHFFFAOYSA-N

Formula: C23H40F4O4

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

Mol. weight [g/mol]: 456.55

Physical Properties

Property code	Value	Unit	Source
gf	-1103.90	kJ/mol	Joback Method
hf	-1806.12	kJ/mol	Joback Method
hfus	62.28	kJ/mol	Joback Method
hvap	80.15	kJ/mol	Joback Method
log10ws	-7.80		Crippen Method
logp	7.235		Crippen Method
mcvol	356.890	ml/mol	McGowan Method
pc	822.42	kPa	Joback Method
rinpol	2546.00		NIST Webbook
rinpol	2546.00		NIST Webbook
tb	871.63	K	Joback Method
tc	1070.25	K	Joback Method
tf	483.07	K	Joback Method
vc	1.427	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1183.87	J/mol×K	871.63	Joback Method
cpg	1203.06	J/mol×K	904.73	Joback Method
cpg	1220.95	J/mol×K	937.84	Joback Method
cpg	1237.61	J/mol×K	970.94	Joback Method
cpg	1253.08	J/mol×K	1004.05	Joback Method
cpg	1267.40	J/mol×K	1037.15	Joback Method
cpg	1280.64	J/mol×K	1070.25	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391653&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

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