Glutaric acid, 2,2,3,3-tetrafluoropropyl 2,4,4-trimethylpentyl ester

Inchi: InChI=1S/C16H26F4O4/c1-11(8-15(2,3)4)9-23-12(21)6-5-7-13(22)24-10-16(19,20)14(17)

InchiKey: WHQACZWNONXVPK-UHFFFAOYSA-N

Formula: C16H26F4O4

SMILES: CC(COC(=O)CCCC(=O)OCC(F)(F)C(F)F)CC(C)(C)C

Mol. weight [g/mol]: 358.37

Physical Properties

Property code	Value	Unit	Source
gf	-1162.44	kJ/mol	Joback Method
hf	-1675.67	kJ/mol	Joback Method
hfus	33.22	kJ/mol	Joback Method
hvap	62.89	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	4.216		Crippen Method
mcvol	258.260	ml/mol	McGowan Method
pc	1286.51	kPa	Joback Method
rinpol	1692.00		NIST Webbook
rinpol	1692.00		NIST Webbook
tb	707.80	K	Joback Method
tc	880.18	K	Joback Method
tf	391.60	K	Joback Method
vc	1.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	769.92	J/mol×K	707.80	Joback Method
cpg	785.52	J/mol×K	736.53	Joback Method
cpg	800.25	J/mol×K	765.26	Joback Method
cpg	814.15	J/mol×K	793.99	Joback Method
cpg	827.24	J/mol×K	822.72	Joback Method
cpg	839.56	J/mol×K	851.45	Joback Method
cpg	851.14	J/mol×K	880.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391523&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