Glutaric acid, oct-1-en-3-yl 2,2,3,3-tetrafluoropropyl ester

Inchi: InChI=1S/C16H24F4O4/c1-3-5-6-8-12(4-2)24-14(22)10-7-9-13(21)23-11-16(19,20)15(17

InchiKey: DINFURYISBXMQS-UHFFFAOYSA-N

Formula: C16H24F4O4

SMILES: C=CC(CCCCC)OC(=O)CCCC(=O)OCC(F)(F)C(F)F

Mol. weight [g/mol]: 356.35

Physical Properties

Property code	Value	Unit	Source
gf	-1077.44	kJ/mol	Joback Method
hf	-1541.49	kJ/mol	Joback Method
hfus	39.35	kJ/mol	Joback Method
hvap	63.51	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	4.278		Crippen Method
mcvol	253.960	ml/mol	McGowan Method
pc	1308.01	kPa	Joback Method
rinpol	1754.00		NIST Webbook
rinpol	1754.00		NIST Webbook
tb	707.71	K	Joback Method
tc	877.07	K	Joback Method
tf	387.42	K	Joback Method
vc	1.010	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	743.39	J/mol×K	707.71	Joback Method
cpg	758.26	J/mol×K	735.94	Joback Method
cpg	772.35	J/mol×K	764.16	Joback Method
cpg	785.67	J/mol×K	792.39	Joback Method
cpg	798.24	J/mol×K	820.61	Joback Method
cpg	810.09	J/mol×K	848.84	Joback Method
cpg	821.24	J/mol×K	877.07	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405344&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