Glutaric acid, 2,2,3,3,4,4,5,5-octafluoropentyl but-3-yn-2-yl ester

Inchi: InChI=1S/C14H14F8O4/c1-3-8(2)26-10(24)6-4-5-9(23)25-7-12(17,18)14(21,22)13(19,20)

InchiKey: DYCBTGNTWMDIMN-UHFFFAOYSA-N

Formula: C14H14F8O4

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

Mol. weight [g/mol]: 398.25

Physical Properties

Property code	Value	Unit	Source
gf	-1732.61	kJ/mol	Joback Method
hf	-2135.68	kJ/mol	Joback Method
hfus	35.92	kJ/mol	Joback Method
hvap	53.73	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	3.436		Crippen Method
mcvol	228.560	ml/mol	McGowan Method
pc	1469.10	kPa	Joback Method
rinpol	1476.00		NIST Webbook
tb	646.01	K	Joback Method
tc	809.44	K	Joback Method
tf	420.81	K	Joback Method
vc	0.928	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	649.11	J/mol×K	646.01	Joback Method
cpg	661.44	J/mol×K	673.25	Joback Method
cpg	673.02	J/mol×K	700.49	Joback Method
cpg	683.88	J/mol×K	727.73	Joback Method
cpg	694.06	J/mol×K	754.97	Joback Method
cpg	703.59	J/mol×K	782.20	Joback Method
cpg	712.51	J/mol×K	809.44	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=U393991&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