Glutaric acid, 2,2,3,3-tetrafluoropropyl 2-methyloct-5-yn-4-yl ester

Inchi: InChI=1S/C17H24F4O4/c1-4-5-7-13(10-12(2)3)25-15(23)9-6-8-14(22)24-11-17(20,21)16

InchiKey: TUNHKAZXFHZQNU-UHFFFAOYSA-N

Formula: C17H24F4O4

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

Mol. weight [g/mol]: 368.36

Physical Properties

Property code	Value	Unit	Source
gf	-956.50	kJ/mol	Joback Method
hf	-1420.54	kJ/mol	Joback Method
hfus	42.82	kJ/mol	Joback Method
hvap	68.17	kJ/mol	Joback Method
log10ws	-4.96		Crippen Method
logp	3.972		Crippen Method
mcvol	263.750	ml/mol	McGowan Method
pc	1336.86	kPa	Joback Method
rinpol	1772.00		NIST Webbook
rinpol	1772.00		NIST Webbook
tb	742.47	K	Joback Method
tc	923.40	K	Joback Method
tf	491.55	K	Joback Method
vc	1.040	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	778.73	J/mol×K	742.47	Joback Method
cpg	793.91	J/mol×K	772.63	Joback Method
cpg	808.21	J/mol×K	802.78	Joback Method
cpg	821.66	J/mol×K	832.94	Joback Method
cpg	834.27	J/mol×K	863.09	Joback Method
cpg	846.07	J/mol×K	893.25	Joback Method
cpg	857.09	J/mol×K	923.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U394015&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