Glutaric acid, but-3-yn-2-yl pentafluorophenyl ester

Inchi: InChI=1S/C15H11F5O4/c1-3-7(2)23-8(21)5-4-6-9(22)24-15-13(19)11(17)10(16)12(18)14

InchiKey: ZXPFAMLOLISZBC-UHFFFAOYSA-N

Formula: C15H11F5O4

SMILES: C#CC(C)OC(=O)CCCC(=O)Oc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 350.24

Physical Properties

Property code	Value	Unit	Source
gf	-1081.58	kJ/mol	Joback Method
hf	-1357.28	kJ/mol	Joback Method
hfus	47.13	kJ/mol	Joback Method
hvap	68.27	kJ/mol	Joback Method
log10ws	-5.14		Crippen Method
logp	3.023		Crippen Method
mcvol	213.580	ml/mol	McGowan Method
pc	1766.90	kPa	Joback Method
rinpol	1676.00		NIST Webbook
rinpol	1676.00		NIST Webbook
tb	732.79	K	Joback Method
tc	919.10	K	Joback Method
tf	527.07	K	Joback Method
vc	0.862	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	579.67	J/mol×K	732.79	Joback Method
cpg	590.68	J/mol×K	763.84	Joback Method
cpg	601.03	J/mol×K	794.89	Joback Method
cpg	610.72	J/mol×K	825.95	Joback Method
cpg	619.75	J/mol×K	857.00	Joback Method
cpg	628.11	J/mol×K	888.05	Joback Method
cpg	635.81	J/mol×K	919.10	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392105&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