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

Inchi: InChI=1S/C16H13F5O4/c1-3-8(2)25-11(23)6-4-5-10(22)24-7-9-12(17)14(19)16(21)15(20

InchiKey: DECBWZCUXWSGDF-UHFFFAOYSA-N

Formula: C16H13F5O4

SMILES: C#CC(C)OC(=O)CCCC(=O)OCc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 364.26

Physical Properties

Property code	Value	Unit	Source
gf	-1073.16	kJ/mol	Joback Method
hf	-1377.92	kJ/mol	Joback Method
hfus	49.72	kJ/mol	Joback Method
hvap	70.49	kJ/mol	Joback Method
log10ws	-5.41		Crippen Method
logp	3.160		Crippen Method
mcvol	227.670	ml/mol	McGowan Method
pc	1632.49	kPa	Joback Method
rinpol	1819.00		NIST Webbook
rinpol	1819.00		NIST Webbook
tb	755.67	K	Joback Method
tc	941.98	K	Joback Method
tf	538.34	K	Joback Method
vc	0.917	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	632.79	J/mol×K	755.67	Joback Method
cpg	644.32	J/mol×K	786.72	Joback Method
cpg	655.14	J/mol×K	817.77	Joback Method
cpg	665.25	J/mol×K	848.83	Joback Method
cpg	674.65	J/mol×K	879.88	Joback Method
cpg	683.33	J/mol×K	910.93	Joback Method
cpg	691.31	J/mol×K	941.98	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391927&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