Glutaric acid, tridec-2-yn-1-yl pentafluorobenzyl ester

Inchi: InChI=1S/C25H31F5O4/c1-2-3-4-5-6-7-8-9-10-11-12-16-33-19(31)14-13-15-20(32)34-17

InchiKey: URFRPWKSSKZZLZ-UHFFFAOYSA-N

Formula: C25H31F5O4

SMILES: CCCCCCCCCCC#CCOC(=O)CCCC(=O)OCc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 490.50

Physical Properties

Property code	Value	Unit	Source
gf	-1015.21	kJ/mol	Joback Method
hf	-1578.00	kJ/mol	Joback Method
hfus	76.70	kJ/mol	Joback Method
hvap	93.21	kJ/mol	Joback Method
log10ws	-9.06		Crippen Method
logp	6.673		Crippen Method
mcvol	354.480	ml/mol	McGowan Method
pc	899.10	kPa	Joback Method
rinpol	2820.00		NIST Webbook
rinpol	2820.00		NIST Webbook
tb	980.91	K	Joback Method
tc	1204.76	K	Joback Method
tf	713.90	K	Joback Method
vc	1.427	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1156.73	J/mol×K	980.91	Joback Method
cpg	1171.81	J/mol×K	1018.22	Joback Method
cpg	1185.34	J/mol×K	1055.53	Joback Method
cpg	1197.32	J/mol×K	1092.84	Joback Method
cpg	1207.80	J/mol×K	1130.14	Joback Method
cpg	1216.77	J/mol×K	1167.45	Joback Method
cpg	1224.28	J/mol×K	1204.76	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391944&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