Glutaric acid, hex-4-yn-3-yl 4-fluoro-2-methoxyphenyl ester

Inchi: InChI=1S/C18H21FO5/c1-4-7-14(5-2)23-17(20)8-6-9-18(21)24-15-11-10-13(19)12-16(15

InchiKey: SHJPKZXVFJVLKY-UHFFFAOYSA-N

Formula: C18H21FO5

SMILES: CC#CC(CC)OC(=O)CCCC(=O)Oc1ccc(F)cc1OC

Mol. weight [g/mol]: 336.35

Physical Properties

Property code	Value	Unit	Source
gf	-373.46	kJ/mol	Joback Method
hf	-752.17	kJ/mol	Joback Method
hfus	45.08	kJ/mol	Joback Method
hvap	80.93	kJ/mol	Joback Method
log10ws	-4.77		Crippen Method
logp	3.255		Crippen Method
mcvol	254.640	ml/mol	McGowan Method
pc	1670.06	kPa	Joback Method
rinpol	2267.00		NIST Webbook
rinpol	2267.00		NIST Webbook
tb	830.71	K	Joback Method
tc	1041.73	K	Joback Method
tf	602.32	K	Joback Method
vc	0.976	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	746.03	J/mol×K	830.71	Joback Method
cpg	760.13	J/mol×K	865.88	Joback Method
cpg	773.09	J/mol×K	901.05	Joback Method
cpg	784.90	J/mol×K	936.22	Joback Method
cpg	795.56	J/mol×K	971.39	Joback Method
cpg	805.07	J/mol×K	1006.56	Joback Method
cpg	813.42	J/mol×K	1041.73	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=U393443&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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