Glutaric acid, but-3-yn-2-yl 2-fluoro-3-trifluoromethylphenyl ester

Inchi: InChI=1S/C16H14F4O4/c1-3-10(2)23-13(21)8-5-9-14(22)24-12-7-4-6-11(15(12)17)16(18

InchiKey: UKGGHFJZIBFUIB-UHFFFAOYSA-N

Formula: C16H14F4O4

SMILES: C#CC(C)OC(=O)CCCC(=O)Oc1cccc(C(F)(F)F)c1F

Mol. weight [g/mol]: 346.27

Physical Properties

Property code	Value	Unit	Source
gf	-846.62	kJ/mol	Joback Method
hf	-1156.15	kJ/mol	Joback Method
hfus	40.39	kJ/mol	Joback Method
hvap	68.03	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	3.485		Crippen Method
mcvol	225.900	ml/mol	McGowan Method
pc	1786.37	kPa	Joback Method
rinpol	1815.00		NIST Webbook
rinpol	1815.00		NIST Webbook
tb	738.23	K	Joback Method
tc	933.96	K	Joback Method
tf	502.61	K	Joback Method
vc	0.888	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	630.91	J/mol×K	738.23	Joback Method
cpg	643.27	J/mol×K	770.85	Joback Method
cpg	654.78	J/mol×K	803.47	Joback Method
cpg	665.47	J/mol×K	836.09	Joback Method
cpg	675.37	J/mol×K	868.71	Joback Method
cpg	684.51	J/mol×K	901.34	Joback Method
cpg	692.92	J/mol×K	933.96	Joback Method

Sources

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=U393614&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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