Glutaric acid, but-3-yn-2-yl 2-bromo-4-fluorophenyl ester

Inchi: InChI=1S/C15H14BrFO4/c1-3-10(2)20-14(18)5-4-6-15(19)21-13-8-7-11(17)9-12(13)16/h1

InchiKey: WXNZDZQNUBXBBE-UHFFFAOYSA-N

Formula: C15H14BrFO4

SMILES: C#CC(C)OC(=O)CCCC(=O)Oc1ccc(F)cc1Br

Mol. weight [g/mol]: 357.17

Physical Properties

Property code	Value	Unit	Source
gf	-259.13	kJ/mol	Joback Method
hf	-512.10	kJ/mol	Joback Method
hfus	41.26	kJ/mol	Joback Method
hvap	75.98	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	3.229		Crippen Method
mcvol	224.000	ml/mol	McGowan Method
pc	2300.32	kPa	Joback Method
rinpol	2072.00		NIST Webbook
tb	786.93	K	Joback Method
tc	1007.53	K	Joback Method
tf	546.95	K	Joback Method
vc	0.852	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	586.72	J/mol×K	786.93	Joback Method
cpg	598.48	J/mol×K	823.70	Joback Method
cpg	609.33	J/mol×K	860.46	Joback Method
cpg	619.30	J/mol×K	897.23	Joback Method
cpg	628.40	J/mol×K	934.00	Joback Method
cpg	636.65	J/mol×K	970.76	Joback Method
cpg	644.08	J/mol×K	1007.53	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391824&Units=SI

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