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

Inchi: InChI=1S/C16H17BrO5/c1-4-11(2)21-15(18)6-5-7-16(19)22-13-9-8-12(17)10-14(13)20-3/

InchiKey: KVIYKGVJSWAXFQ-UHFFFAOYSA-N

Formula: C16H17BrO5

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

Mol. weight [g/mol]: 369.21

Physical Properties

Property code	Value	Unit	Source
gf	-160.90	kJ/mol	Joback Method
hf	-468.85	kJ/mol	Joback Method
hfus	41.96	kJ/mol	Joback Method
hvap	81.44	kJ/mol	Joback Method
log10ws	-4.77		Crippen Method
logp	3.098		Crippen Method
mcvol	242.190	ml/mol	McGowan Method
pc	2157.31	kPa	Joback Method
rinpol	2348.00		NIST Webbook
rinpol	2348.00		NIST Webbook
tb	832.96	K	Joback Method
tc	1056.86	K	Joback Method
tf	579.86	K	Joback Method
vc	0.907	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	659.10	J/mol×K	832.96	Joback Method
cpg	671.32	J/mol×K	870.28	Joback Method
cpg	682.49	J/mol×K	907.59	Joback Method
cpg	692.61	J/mol×K	944.91	Joback Method
cpg	701.69	J/mol×K	982.23	Joback Method
cpg	709.72	J/mol×K	1019.55	Joback Method
cpg	716.74	J/mol×K	1056.86	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=U393661&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