Glutaric acid, hex-4-yn-3-yl 4-bromophenyl ester

Inchi: InChI=1S/C17H19BrO4/c1-3-6-14(4-2)21-16(19)7-5-8-17(20)22-15-11-9-13(18)10-12-15/

InchiKey: XDBCSDVGZSIQAW-UHFFFAOYSA-N

Formula: C17H19BrO4

SMILES: CC#CC(CC)OC(=O)CCCC(=O)Oc1ccc(Br)cc1

Mol. weight [g/mol]: 367.23

Physical Properties

Property code	Value	Unit	Source
gf	-58.12	kJ/mol	Joback Method
hf	-365.40	kJ/mol	Joback Method
hfus	43.90	kJ/mol	Joback Method
hvap	82.89	kJ/mol	Joback Method
log10ws	-5.48		Crippen Method
logp	3.870		Crippen Method
mcvol	250.410	ml/mol	McGowan Method
pc	2056.76	kPa	Joback Method
rinpol	2441.00		NIST Webbook
rinpol	2441.00		NIST Webbook
tb	847.32	K	Joback Method
tc	1077.29	K	Joback Method
tf	615.51	K	Joback Method
vc	0.946	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	692.19	J/mol×K	847.32	Joback Method
cpg	705.44	J/mol×K	885.65	Joback Method
cpg	717.55	J/mol×K	923.98	Joback Method
cpg	728.56	J/mol×K	962.30	Joback Method
cpg	738.49	J/mol×K	1000.63	Joback Method
cpg	747.37	J/mol×K	1038.96	Joback Method
cpg	755.22	J/mol×K	1077.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393290&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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