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

Inchi: InChI=1S/C18H21BrO5/c1-4-7-14(5-2)23-17(20)8-6-9-18(21)24-15-11-10-13(19)12-16(15

InchiKey: LLHRVXGEBHWNKA-UHFFFAOYSA-N

Formula: C18H21BrO5

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

Mol. weight [g/mol]: 397.26

Physical Properties

Property code	Value	Unit	Source
gf	-164.33	kJ/mol	Joback Method
hf	-529.73	kJ/mol	Joback Method
hfus	47.28	kJ/mol	Joback Method
hvap	88.18	kJ/mol	Joback Method
log10ws	-5.60		Crippen Method
logp	3.878		Crippen Method
mcvol	270.370	ml/mol	McGowan Method
pc	1837.26	kPa	Joback Method
rinpol	2589.00		NIST Webbook
rinpol	2589.00		NIST Webbook
tb	897.60	K	Joback Method
tc	1124.76	K	Joback Method
tf	661.53	K	Joback Method
vc	1.020	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	773.96	J/mol×K	897.60	Joback Method
cpg	786.65	J/mol×K	935.46	Joback Method
cpg	798.08	J/mol×K	973.32	Joback Method
cpg	808.26	J/mol×K	1011.18	Joback Method
cpg	817.17	J/mol×K	1049.04	Joback Method
cpg	824.84	J/mol×K	1086.90	Joback Method
cpg	831.26	J/mol×K	1124.76	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393886&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

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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