Glutaric acid, tridec-2-yn-1-yl 4-bromo-2-methoxyphenyl ester

Inchi: InChI=1S/C25H35BrO5/c1-3-4-5-6-7-8-9-10-11-12-13-19-30-24(27)15-14-16-25(28)31-22

InchiKey: AREHECRSKFGMPR-UHFFFAOYSA-N

Formula: C25H35BrO5

SMILES: CCCCCCCCCCC#CCOC(=O)CCCC(=O)Oc1ccc(Br)cc1OC

Mol. weight [g/mol]: 495.45

Physical Properties

Property code	Value	Unit	Source
gf	-102.95	kJ/mol	Joback Method
hf	-668.93	kJ/mol	Joback Method
hfus	68.94	kJ/mol	Joback Method
hvap	104.15	kJ/mol	Joback Method
log10ws	-8.42		Crippen Method
logp	6.611		Crippen Method
mcvol	369.000	ml/mol	McGowan Method
pc	1101.54	kPa	Joback Method
rinpol	3369.00		NIST Webbook
tb	1058.20	K	Joback Method
tc	1295.54	K	Joback Method
tf	755.42	K	Joback Method
vc	1.417	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1188.37	J/mol×K	1058.20	Joback Method
cpg	1201.46	J/mol×K	1097.76	Joback Method
cpg	1212.87	J/mol×K	1137.31	Joback Method
cpg	1222.63	J/mol×K	1176.87	Joback Method
cpg	1230.78	J/mol×K	1216.43	Joback Method
cpg	1237.35	J/mol×K	1255.99	Joback Method
cpg	1242.37	J/mol×K	1295.54	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393896&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