Glutaric acid, tridec-2-yn-1-yl 4-bromophenyl ester

Inchi: InChI=1S/C24H33BrO4/c1-2-3-4-5-6-7-8-9-10-11-12-20-28-23(26)14-13-15-24(27)29-22-
InchiKey: IZFRFWDOJNWWRK-UHFFFAOYSA-N
Formula: C24H33BrO4
SMILES: CCCCCCCCCCC#CCOC(=O)CCCC(=O)Oc1ccc(Br)cc1
Mol. weight [g/mol]: 465.42

Physical Properties

Property code	Value	Unit	Source
gf	3.26	kJ/mol	Joback Method
hf	-504.60	kJ/mol	Joback Method
hfus	65.55	kJ/mol	Joback Method
hvap	98.85	kJ/mol	Joback Method
log10ws	-8.30		Crippen Method
logp	6.602		Crippen Method
mcvol	349.040	ml/mol	McGowan Method
pc	1201.46	kPa	Joback Method
rinpol	3253.00		NIST Webbook
rinpol	3253.00		NIST Webbook
tb	1007.92	K	Joback Method
tc	1235.77	K	Joback Method
tf	709.40	K	Joback Method
vc	1.343	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1102.08	J/mol×K	1007.92	Joback Method
cpg	1116.33	J/mol×K	1045.89	Joback Method
cpg	1129.25	J/mol×K	1083.87	Joback Method
cpg	1140.89	J/mol×K	1121.84	Joback Method
cpg	1151.29	J/mol×K	1159.82	Joback Method
cpg	1160.53	J/mol×K	1197.79	Joback Method
cpg	1168.63	J/mol×K	1235.77	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=U393300&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