4-Butylbenzoic acid, dodec-9-ynyl ester

Inchi: InChI=1S/C23H34O2/c1-3-5-7-8-9-10-11-12-13-14-20-25-23(24)22-18-16-21(17-19-22)1
InchiKey: FRMKCYYFFDURBJ-UHFFFAOYSA-N
Formula: C23H34O2
SMILES: CCC#CCCCCCCCCOC(=O)c1ccc(CCCC)cc1
Mol. weight [g/mol]: 342.51

Physical Properties

Property code	Value	Unit	Source
gf	214.44	kJ/mol	Joback Method
hf	-265.49	kJ/mol	Joback Method
hfus	54.89	kJ/mol	Joback Method
hvap	81.04	kJ/mol	Joback Method
log10ws	-7.75		Crippen Method
logp	6.330		Crippen Method
mcvol	310.010	ml/mol	McGowan Method
pc	1185.79	kPa	Joback Method
rinpol	2522.50		NIST Webbook
rinpol	2522.50		NIST Webbook
tb	842.59	K	Joback Method
tc	1046.31	K	Joback Method
tf	566.17	K	Joback Method
vc	1.202	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	955.57	J/mol×K	842.59	Joback Method
cpg	973.82	J/mol×K	876.54	Joback Method
cpg	990.92	J/mol×K	910.50	Joback Method
cpg	1006.90	J/mol×K	944.45	Joback Method
cpg	1021.81	J/mol×K	978.41	Joback Method
cpg	1035.69	J/mol×K	1012.36	Joback Method
cpg	1048.58	J/mol×K	1046.31	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292211&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