Benzeneacetic acid, 4-chloro-, tridec-2-yn-1-yl ester

Inchi: InChI=1S/C21H29ClO2/c1-2-3-4-5-6-7-8-9-10-11-12-17-24-21(23)18-19-13-15-20(22)16-

InchiKey: YUBBPVFTUZYXFF-UHFFFAOYSA-N

Formula: C21H29ClO2

SMILES: CCCCCCCCCCC#CCOC(=O)Cc1ccc(Cl)cc1

Mol. weight [g/mol]: 348.91

Physical Properties

Property code	Value	Unit	Source
gf	185.67	kJ/mol	Joback Method
hf	-239.95	kJ/mol	Joback Method
hfus	53.90	kJ/mol	Joback Method
hvap	80.97	kJ/mol	Joback Method
log10ws	-7.06		Crippen Method
logp	5.960		Crippen Method
mcvol	294.070	ml/mol	McGowan Method
pc	1323.28	kPa	Joback Method
rinpol	2608.00		NIST Webbook
rinpol	2608.00		NIST Webbook
tb	834.26	K	Joback Method
tc	1042.88	K	Joback Method
tf	573.55	K	Joback Method
vc	1.139	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	865.70	J/mol×K	834.26	Joback Method
cpg	882.42	J/mol×K	869.03	Joback Method
cpg	898.03	J/mol×K	903.80	Joback Method
cpg	912.59	J/mol×K	938.57	Joback Method
cpg	926.12	J/mol×K	973.34	Joback Method
cpg	938.69	J/mol×K	1008.11	Joback Method
cpg	950.31	J/mol×K	1042.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407003&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