Phenylacetic acid, tridec-2-ynyl ester

Inchi: InChI=1S/C21H30O2/c1-2-3-4-5-6-7-8-9-10-11-15-18-23-21(22)19-20-16-13-12-14-17-20
InchiKey: JMGAKRHSWMRTAM-UHFFFAOYSA-N
Formula: C21H30O2
SMILES: CCCCCCCCCCC#CCOC(=O)Cc1ccccc1
Mol. weight [g/mol]: 314.46

Physical Properties

Property code	Value	Unit	Source
gf	207.23	kJ/mol	Joback Method
hf	-212.74	kJ/mol	Joback Method
hfus	50.10	kJ/mol	Joback Method
hvap	75.92	kJ/mol	Joback Method
log10ws	-6.37		Crippen Method
logp	5.306		Crippen Method
mcvol	281.830	ml/mol	McGowan Method
pc	1374.80	kPa	Joback Method
rinpol	2376.10		NIST Webbook
rinpol	2376.10		NIST Webbook
tb	791.85	K	Joback Method
tc	995.57	K	Joback Method
tf	531.11	K	Joback Method
vc	1.089	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	836.95	J/mol×K	791.85	Joback Method
cpg	854.94	J/mol×K	825.80	Joback Method
cpg	871.82	J/mol×K	859.76	Joback Method
cpg	887.62	J/mol×K	893.71	Joback Method
cpg	902.39	J/mol×K	927.66	Joback Method
cpg	916.17	J/mol×K	961.62	Joback Method
cpg	929.00	J/mol×K	995.57	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292538&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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