Carbonic acid, but-2-yn-1-yl eicosyl ester

Inchi: InChI=1S/C25H46O3/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-24-28-25(2
InchiKey: MNDFUBOBECJYKH-UHFFFAOYSA-N
Formula: C25H46O3
SMILES: CC#CCOC(=O)OCCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 394.63

Physical Properties

Property code	Value	Unit	Source
gf	23.50	kJ/mol	Joback Method
hf	-664.05	kJ/mol	Joback Method
hfus	67.60	kJ/mol	Joback Method
hvap	84.96	kJ/mol	Joback Method
log10ws	-9.01		Crippen Method
logp	8.205		Crippen Method
mcvol	367.820	ml/mol	McGowan Method
pc	850.48	kPa	Joback Method
rinpol	2817.00		NIST Webbook
rinpol	2817.00		NIST Webbook
tb	879.11	K	Joback Method
tc	1076.28	K	Joback Method
tf	572.00	K	Joback Method
vc	1.440	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1204.11	J/mol×K	879.11	Joback Method
cpg	1224.83	J/mol×K	911.97	Joback Method
cpg	1244.24	J/mol×K	944.83	Joback Method
cpg	1262.39	J/mol×K	977.69	Joback Method
cpg	1279.30	J/mol×K	1010.56	Joback Method
cpg	1295.00	J/mol×K	1043.42	Joback Method
cpg	1309.52	J/mol×K	1076.28	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=U383214&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

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