Carbonic acid, heptadecyl prop-1-en-2-yl ester

Inchi: InChI=1S/C21H40O3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-23-21(22)24-20(2)3
InchiKey: NWBQIQOVPQVSKK-UHFFFAOYSA-N
Formula: C21H40O3
SMILES: C=C(C)OC(=O)OCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 340.54

Physical Properties

Property code	Value	Unit	Source
gf	-133.69	kJ/mol	Joback Method
hf	-738.15	kJ/mol	Joback Method
hfus	51.53	kJ/mol	Joback Method
hvap	73.32	kJ/mol	Joback Method
log10ws	-7.89		Crippen Method
logp	7.545		Crippen Method
mcvol	315.760	ml/mol	McGowan Method
pc	1002.71	kPa	Joback Method
rinpol	2287.00		NIST Webbook
tb	775.15	K	Joback Method
tc	952.83	K	Joback Method
tf	405.10	K	Joback Method
vc	1.236	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	975.84	J/mol×K	775.15	Joback Method
cpg	995.33	J/mol×K	804.76	Joback Method
cpg	1013.83	J/mol×K	834.38	Joback Method
cpg	1031.36	J/mol×K	863.99	Joback Method
cpg	1047.93	J/mol×K	893.60	Joback Method
cpg	1063.58	J/mol×K	923.22	Joback Method
cpg	1078.32	J/mol×K	952.83	Joback Method

Sources

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=U382902&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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