

Carbonic acid, but-3-en-1-yl eicosyl ester

Inchi: InChI=1S/C25H48O3/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-24-28-25(2
InchiKey: UFWMGBPQKPMGKI-UHFFFAOYSA-N
Formula: C25H48O3
SMILES: C=CCCOC(=O)OCCCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 396.65

Physical Properties

Property code	Value	Unit	Source
gf	-91.46	kJ/mol	Joback Method
hf	-810.92	kJ/mol	Joback Method
hfus	63.20	kJ/mol	Joback Method
hvap	82.14	kJ/mol	Joback Method
log10ws	-9.07		Crippen Method
logp	8.757		Crippen Method
mvol	372.120	ml/mol	McGowan Method
pc	794.84	kPa	Joback Method
rinpol	2710.00		NIST Webbook
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tb	866.79	K	Joback Method
tc	1061.96	K	Joback Method
tf	464.14	K	Joback Method
vc	1.458	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1226.54	J/mol×K	866.79	Joback Method
cpg	1248.08	J/mol×K	899.32	Joback Method
cpg	1268.31	J/mol×K	931.85	Joback Method
cpg	1287.26	J/mol×K	964.38	Joback Method
cpg	1304.99	J/mol×K	996.90	Joback Method
cpg	1321.52	J/mol×K	1029.43	Joback Method
cpg	1336.89	J/mol×K	1061.96	Joback Method
dvisc	0.0006342	Paxs	464.14	Joback Method

dvisc	0.0002735	Paxs	531.25	Joback Method
dvisc	0.0001425	Paxs	598.36	Joback Method
dvisc	0.0000846	Paxs	665.46	Joback Method
dvisc	0.0000553	Paxs	732.57	Joback Method
dvisc	0.0000388	Paxs	799.68	Joback Method
dvisc	0.0000288	Paxs	866.79	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U383240&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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