

Citric acid, triallyl ester

Other names:	triallyl citrate
Inchi:	InChI=1S/C15H20O7/c1-4-7-20-12(16)10-15(19,14(18)22-9-6-3)11-13(17)21-8-5-2/h4-6,
InchiKey:	PLCFYBDYBCOLSP-UHFFFAOYSA-N
Formula:	C15H20O7
SMILES:	C=CCOC(=O)CC(O)(CC(=O)OCC=C)C(=O)OCC=C
Mol. weight [g/mol]:	312.32
CAS:	6299-73-6

Physical Properties

Property code	Value	Unit	Source
gf	-496.80	kJ/mol	Joback Method
hf	-872.02	kJ/mol	Joback Method
hfus	35.80	kJ/mol	Joback Method
hvap	89.82	kJ/mol	Joback Method
log10ws	-1.63		Crippen Method
logp	0.685		Crippen Method
mcvol	237.500	ml/mol	McGowan Method
pc	1918.62	kPa	Joback Method
tb	850.46	K	Joback Method
tc	1047.52	K	Joback Method
tf	533.25	K	Joback Method
vc	0.898	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	706.98	J/mol×K	850.46	Joback Method
cpg	717.94	J/mol×K	883.30	Joback Method
cpg	728.07	J/mol×K	916.15	Joback Method
cpg	737.40	J/mol×K	948.99	Joback Method
cpg	745.95	J/mol×K	981.83	Joback Method
cpg	753.75	J/mol×K	1014.68	Joback Method
cpg	760.80	J/mol×K	1047.52	Joback Method
dvisc	0.0002911	Pa×s	533.25	Joback Method

dvisc	0.0001338	Pa×s	586.12	Joback Method
dvisc	0.0000700	Pa×s	638.99	Joback Method
dvisc	0.0000404	Pa×s	691.86	Joback Method
dvisc	0.0000252	Pa×s	744.72	Joback Method
dvisc	0.0000168	Pa×s	797.59	Joback Method
dvisc	0.0000117	Pa×s	850.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6299736&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
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:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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