1-Propene-1,2,3-tricarboxylic acid, tributyl ester

Other names: Tributyl aconitate
Tri-n-butyl aconitate
1-Propene-1,2,3-tricarboxylic acid, tris(N.-butyl ester)
1,2,3-Propenetricarboxylic acid, tributyl ester
Tributyl (1z)-1-propene-1,2,3-tricarboxylate
tributyl prop-1-ene-1,2,3-tricarboxylate
trans aconitic acid, tributyl ester

Inchi: InChI=1S/C18H30O6/c1-4-7-10-22-16(19)13-15(18(21)24-12-9-6-3)14-17(20)23-11-8-5-2

InchiKey: BANLNYYTSYHBAP-SQFISAMPSA-N

Formula: C18H30O6

SMILES: CCCCOC(=O)C=C(CC(=O)OCCCC)C(=O)OCCCC

Mol. weight [g/mol]: 342.43

CAS: 7568-58-3

Physical Properties

Property code	Value	Unit	Source
gf	-529.41	kJ/mol	Joback Method
hf	-1041.82	kJ/mol	Joback Method
hfus	49.63	kJ/mol	Joback Method
hvap	83.17	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	3.333		Crippen Method
mcvol	282.500	ml/mol	McGowan Method
pc	1321.35	kPa	Joback Method
tb	844.15	K	Joback Method
tc	1038.39	K	Joback Method
tf	490.06	K	Joback Method
vc	1.097	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	875.43	J/mol×K	844.15	Joback Method
cpg	890.72	J/mol×K	876.52	Joback Method

cpg	904.98	J/mol×K	908.90	Joback Method
cpg	918.22	J/mol×K	941.27	Joback Method
cpg	930.45	J/mol×K	973.65	Joback Method
cpg	941.68	J/mol×K	1006.02	Joback Method
cpg	951.93	J/mol×K	1038.39	Joback Method
hvapt	87.40	kJ/mol	434.00	NIST Webbook

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=C7568583&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
hvapt:	Enthalpy of vaporization at a given temperature
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