benzoic acid, 3,4,5-trihydroxy-, octyl ester

Other names: gallic acid, octyl ester
octyl gallate
Inchi: InChI=1S/C15H22O5/c1-2-3-4-5-6-7-8-20-15(19)11-9-12(16)14(18)13(17)10-11/h9-10,16
InchiKey: NRPKURNSADTHLJ-UHFFFAOYSA-N
Formula: C15H22O5
SMILES: CCCCCCCCOC(=O)c1cc(O)c(O)c(O)c1
Mol. weight [g/mol]: 282.34

Physical Properties

Property code	Value	Unit	Source
af	1.1305		Cheméo Relay (1.0)
hf	-941.92	kJ/mol	Cheméo Relay (1.0)
hfus	48.78	kJ/mol	Joback Method
hvap	130.61	kJ/mol	Cheméo Relay (1.0)
log10ws	-3.86		Cheméo Relay (1.0)
logp	3.321		Crippen Method
mcvol	223.500	ml/mol	McGowan Method
pc	2973.04	kPa	Joback Method
tb	628.26	K	Cheméo Relay (1.0)
tc	880.46	K	Cheméo Relay (1.0)
tf	385.32	K	Cheméo Relay (1.0)
vc	0.815	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	707.27	J/mol×K	887.43	Joback Method
cpg	721.20	J/mol×K	924.78	Joback Method
cpg	735.14	J/mol×K	962.13	Joback Method
cpg	749.25	J/mol×K	999.48	Joback Method
cpg	763.70	J/mol×K	1036.82	Joback Method
cpg	778.65	J/mol×K	1074.17	Joback Method
cpg	794.27	J/mol×K	1111.52	Joback Method
dvisc	0.0000003	Pa×s	692.55	Joback Method

dvisc	0.0000001	Pa×s	725.03	Joback Method
dvisc	7.9397948e-08	Pa×s	757.51	Joback Method
dvisc	4.6993636e-08	Pa×s	789.99	Joback Method
dvisc	2.8990685e-08	Pa×s	822.47	Joback Method
dvisc	1.8553133e-08	Pa×s	854.95	Joback Method
dvisc	1.2267759e-08	Pa×s	887.43	Joback Method

Sources

Cheméo Relay (1.0, beta):

Solubilities of Gallic Acid and Its Esters in Water: https://www.doi.org/10.1021/je0601661

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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