3,5-DI-T-BUTYLBENZOIC ACID

Other names: 3,5-bis(tert-butyl)benzoic acid
3,5-di-tert-butylbenzoic acid
Benzoic acid, 3,5-bis(1,1-dimethylethyl)-
Inchi: InChI=1S/C15H22O2/c1-14(2,3)11-7-10(13(16)17)8-12(9-11)15(4,5)6/h7-9H,1-6H3,(H,16
InchiKey: NCTSLPBQVXUAHR-UHFFFAOYSA-N
Formula: C15H22O2
SMILES: CC(C)(C)c1cc(C(=O)O)cc(C(C)(C)C)c1
Mol. weight [g/mol]: 234.34
CAS: 16225-26-6

Physical Properties

Property code	Value	Unit	Source
chs	-8422.10 ± 1.40	kJ/mol	NIST Webbook
hf	-516.30 ± 1.90	kJ/mol	NIST Webbook
hfs	-624.60 ± 1.60	kJ/mol	NIST Webbook
hfus	18.73	kJ/mol	Joback Method
hsub	108.30	kJ/mol	NIST Webbook
hvap	98.41	kJ/mol	Cheméo Relay (1.0)
ie	8.73	eV	Cheméo Relay (1.0)
log10ws	-4.96		Cheméo Relay (1.0)
logp	3.980		Crippen Method
mcvol	205.890	ml/mol	McGowan Method
tb	559.91	K	Cheméo Relay (1.0)
tf	468.96	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	659.21	J/mol×K	927.74	Joback Method
cpg	637.54	J/mol×K	858.10	Joback Method
cpg	584.75	J/mol×K	718.83	Joback Method
cpg	599.31	J/mol×K	753.65	Joback Method
cpg	612.91	J/mol×K	788.47	Joback Method
cpg	625.63	J/mol×K	823.28	Joback Method

cpg	648.71	J/mol×K	892.92	Joback Method
dvisc	0.0013696	Pa×s	425.86	Joback Method
dvisc	0.0005087	Pa×s	474.69	Joback Method
dvisc	0.0002273	Pa×s	523.52	Joback Method
dvisc	0.0001165	Pa×s	572.35	Joback Method
dvisc	0.0000663	Pa×s	621.17	Joback Method
dvisc	0.0000410	Pa×s	670.00	Joback Method
dvisc	0.0000271	Pa×s	718.83	Joback Method
hsubt	108.40 ± 4.20	kJ/mol	348.00	NIST Webbook
hsubt	108.40 ± 0.50	kJ/mol	348.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.22933e+01
Coeff. B	-4.10588e+03
Coeff. C	-9.96100e+01
Temperature range (K), min.	441.61
Temperature range (K), max.	687.70

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C16225266&Units=SI
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):
Cheméo Relay (1.0, beta):

Legend

chs: Standard solid enthalpy of combustion

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point