

1,2,4-Benzenetriol, tributyrate

Inchi:	InChI=1S/C18H24O6/c1-4-7-16(19)22-13-10-11-14(23-17(20)8-5-2)15(12-13)24-18(21)9
InchiKey:	RBRYTTOGADCOGW-UHFFFAOYSA-N
Formula:	C18H24O6
SMILES:	CCCC(=O)Oc1ccc(OC(=O)CCC)c(OC(=O)CCC)c1
Mol. weight [g/mol]:	336.38
CAS:	111443-88-0

Physical Properties

Property code	Value	Unit	Source
gf	-507.93	kJ/mol	Joback Method
hf	-935.66	kJ/mol	Joback Method
hfus	44.00	kJ/mol	Joback Method
hvap	86.73	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	3.803		Crippen Method
mcvol	263.040	ml/mol	McGowan Method
pc	1591.08	kPa	Joback Method
tb	876.75	K	Joback Method
tc	1085.35	K	Joback Method
tf	560.56	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	804.17	J/molxK	876.75	Joback Method
cpg	858.65	J/molxK	1050.59	Joback Method
cpg	850.17	J/molxK	1015.82	Joback Method
cpg	840.49	J/molxK	981.05	Joback Method
cpg	829.59	J/molxK	946.28	Joback Method
cpg	817.48	J/molxK	911.52	Joback Method
cpg	865.90	J/molxK	1085.35	Joback Method
dvisc	0.0000531	Paxs	876.75	Joback Method
dvisc	0.0000662	Paxs	824.05	Joback Method

dvisc	0.0000852	Paxs	771.35	Joback Method
dvisc	0.0001138	Paxs	718.65	Joback Method
dvisc	0.0001590	Paxs	665.96	Joback Method
dvisc	0.0002355	Paxs	613.26	Joback Method
dvisc	0.0003753	Paxs	560.56	Joback Method

Sources

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=C111443880&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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