1-Bromo-2,4,6-triisopropylbenzene

Inchi: InChI=1S/C15H23Br/c1-9(2)12-7-13(10(3)4)15(16)14(8-12)11(5)6/h7-11H,1-6H3
InchiKey: FUMMYHVKFAHQST-UHFFFAOYSA-N
Formula: C15H23Br
SMILES: CC(C)c1cc(C(C)C)c(Br)c(C(C)C)c1
Mol. weight [g/mol]: 283.25
CAS: 21524-34-5

Physical Properties

Property code	Value	Unit	Source
gf	165.94	kJ/mol	Joback Method
hf	-140.32	kJ/mol	Joback Method
hfus	22.20	kJ/mol	Joback Method
hvap	58.52	kJ/mol	Joback Method
log10ws	-6.19		Crippen Method
logp	5.819		Crippen Method
mcvol	215.950	ml/mol	McGowan Method
pc	1925.36	kPa	Joback Method
tb	649.06	K	Joback Method
tc	867.42	K	Joback Method
tf	337.59	K	Joback Method
vc	0.811	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	542.99	J/mol×K	649.06	Joback Method
cpg	560.83	J/mol×K	685.45	Joback Method
cpg	577.63	J/mol×K	721.85	Joback Method
cpg	593.43	J/mol×K	758.24	Joback Method
cpg	608.27	J/mol×K	794.63	Joback Method
cpg	622.21	J/mol×K	831.02	Joback Method
cpg	635.27	J/mol×K	867.42	Joback Method
dvisc	0.0020784	Pa×s	337.59	Joback Method
dvisc	0.0009434	Pa×s	389.50	Joback Method

dvisc	0.0005156	Pa×s	441.41	Joback Method
dvisc	0.0003200	Pa×s	493.32	Joback Method
dvisc	0.0002175	Pa×s	545.24	Joback Method
dvisc	0.0001581	Pa×s	597.15	Joback Method
dvisc	0.0001209	Pa×s	649.06	Joback Method

Sources

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=C21524345&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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