4,5-Dibromo-o-xylene

Other names: 4,5-Dibromo-o-xylene
Inchi: InChI=1S/C8H8Br2/c1-5-3-7(9)8(10)4-6(5)2/h3-4H,1-2H3
InchiKey: BCIDDURGCAHERU-UHFFFAOYSA-N
Formula: C8H8Br2
SMILES: Cc1cc(Br)c(Br)cc1C
Mol. weight [g/mol]: 263.96

Physical Properties

Property code	Value	Unit	Source
af	0.4210		Cheméo Relay (1.0)
gf	128.64	kJ/mol	Joback Method
hf	65.27	kJ/mol	Cheméo Relay (1.0)
hfus	19.92	kJ/mol	Joback Method
ie	8.41	eV	Cheméo Relay (1.0)
log10ws	-5.37		Cheméo Relay (1.0)
logp	3.828		Crippen Method
mcvol	134.820	ml/mol	McGowan Method
pc	4098.62	kPa	Joback Method
tb	551.20	K	NIST Webbook
tc	748.42	K	Cheméo Relay (1.0)
tf	363.82	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	244.05	J/mol×K	556.38	Joback Method
cpg	294.83	J/mol×K	804.69	Joback Method
cpg	287.79	J/mol×K	763.31	Joback Method
cpg	280.23	J/mol×K	721.92	Joback Method
cpg	272.13	J/mol×K	680.54	Joback Method
cpg	263.42	J/mol×K	639.15	Joback Method
cpg	254.08	J/mol×K	597.77	Joback Method
dvisc	0.0004971	Pa×s	459.94	Joback Method
dvisc	0.0002810	Pa×s	556.38	Joback Method

dvisc	0.0003320	Pa×s	524.23	Joback Method
dvisc	0.0004009	Pa×s	492.09	Joback Method
dvisc	0.0011896	Pa×s	363.50	Joback Method
dvisc	0.0006364	Pa×s	427.79	Joback Method
dvisc	0.0008483	Pa×s	395.65	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C24932487&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

Legend

af: Acentric Factor
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
ie: Ionization energy
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