2-Bromobenzoic acid, 4-benzyloxyphenyl ester

Inchi: InChI=1S/C20H15BrO3/c21-19-9-5-4-8-18(19)20(22)24-17-12-10-16(11-13-17)23-14-15-

InchiKey: JKZQAEUUZDABPS-UHFFFAOYSA-N

Formula: C20H15BrO3

SMILES: O=C(Oc1ccc(OCc2ccccc2)cc1)c1ccccc1Br

Mol. weight [g/mol]: 383.24

Physical Properties

Property code	Value	Unit	Source
gf	110.89	kJ/mol	Joback Method
hf	-120.17	kJ/mol	Joback Method
hfus	38.16	kJ/mol	Joback Method
hvap	86.27	kJ/mol	Joback Method
log10ws	-6.95		Crippen Method
logp	5.247		Crippen Method
mcvol	252.190	ml/mol	McGowan Method
pc	2318.07	kPa	Joback Method
rinpol	2929.00		NIST Webbook
rinpol	2929.00		NIST Webbook
tb	911.87	K	Joback Method
tc	1174.23	K	Joback Method
tf	573.65	K	Joback Method
vc	0.935	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	701.50	J/mol×K	911.87	Joback Method
cpg	713.67	J/mol×K	955.60	Joback Method
cpg	724.43	J/mol×K	999.32	Joback Method
cpg	733.85	J/mol×K	1043.05	Joback Method
cpg	742.03	J/mol×K	1086.78	Joback Method
cpg	749.05	J/mol×K	1130.51	Joback Method
cpg	754.99	J/mol×K	1174.23	Joback Method
dvisc	0.0003331	Pa×s	573.65	Joback Method

dvisc	0.0002097	Pa×s	630.02	Joback Method
dvisc	0.0001425	Pa×s	686.39	Joback Method
dvisc	0.0001026	Pa×s	742.76	Joback Method
dvisc	0.0000774	Pa×s	799.13	Joback Method
dvisc	0.0000606	Pa×s	855.50	Joback Method
dvisc	0.0000489	Pa×s	911.87	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=U307750&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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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