1,2-Cyclohexanedicarboxylic acid, 4-bromophenyl decyl ester

Inchi: InChI=1S/C24H35BrO4/c1-2-3-4-5-6-7-8-11-18-28-23(26)21-12-9-10-13-22(21)24(27)29-

InchiKey: QQTZLRDAGYQWRA-UHFFFAOYSA-N

Formula: C24H35BrO4

SMILES: CCCCCCCCCCOC(=O)C1CCCCC1C(=O)Oc1ccc(Br)cc1

Mol. weight [g/mol]: 467.44

Physical Properties

Property code	Value	Unit	Source
gf	-182.80	kJ/mol	Joback Method
hf	-742.92	kJ/mol	Joback Method
hfus	55.33	kJ/mol	Joback Method
hvap	96.82	kJ/mol	Joback Method
log10ws	-7.92		Crippen Method
logp	6.845		Crippen Method
mcvol	346.780	ml/mol	McGowan Method
pc	1211.51	kPa	Joback Method
rinpol	3159.00		NIST Webbook
rinpol	3159.00		NIST Webbook
tb	1013.80	K	Joback Method
tc	1244.93	K	Joback Method
tf	606.44	K	Joback Method
vc	1.313	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1157.45	J/mol×K	1013.80	Joback Method
cpg	1172.06	J/mol×K	1052.32	Joback Method
cpg	1184.99	J/mol×K	1090.84	Joback Method
cpg	1196.28	J/mol×K	1129.36	Joback Method
cpg	1205.99	J/mol×K	1167.88	Joback Method
cpg	1214.18	J/mol×K	1206.40	Joback Method
cpg	1220.90	J/mol×K	1244.93	Joback Method
dvisc	0.0003162	Pa×s	606.44	Joback Method

dvisc	0.0001783	Pa×s	674.33	Joback Method
dvisc	0.0001117	Pa×s	742.23	Joback Method
dvisc	0.0000756	Pa×s	810.12	Joback Method
dvisc	0.0000544	Pa×s	878.01	Joback Method
dvisc	0.0000410	Pa×s	945.91	Joback Method
dvisc	0.0000321	Pa×s	1013.80	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=U339633&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