

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

Inchi:	InChI=1S/C21H29BrO4/c1-2-3-4-5-8-15-25-20(23)18-9-6-7-10-19(18)21(24)26-17-13-11
InchiKey:	OMQLBDFPDGIKRT-UHFFFAOYSA-N
Formula:	C21H29BrO4
SMILES:	CCCCCCCOC(=O)C1CCCCC1C(=O)Oc1ccc(Br)cc1
Mol. weight [g/mol]:	425.36

Physical Properties

Property code	Value	Unit	Source
gf	-208.06	kJ/mol	Joback Method
hf	-681.00	kJ/mol	Joback Method
hfus	47.56	kJ/mol	Joback Method
hvap	90.14	kJ/mol	Joback Method
log10ws	-6.66		Crippen Method
logp	5.675		Crippen Method
mcvol	304.510	ml/mol	McGowan Method
pc	1496.51	kPa	Joback Method
rinpol	2835.00		NIST Webbook
tb	945.16	K	Joback Method
tc	1173.37	K	Joback Method
tf	572.63	K	Joback Method
vc	1.145	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	976.05	J/molxK	945.16	Joback Method
cpg	990.94	J/molxK	983.20	Joback Method
cpg	1004.26	J/molxK	1021.23	Joback Method
cpg	1016.04	J/molxK	1059.27	Joback Method
cpg	1026.33	J/molxK	1097.30	Joback Method
cpg	1035.16	J/molxK	1135.34	Joback Method
cpg	1042.58	J/molxK	1173.37	Joback Method
dvisc	0.0004466	Paxs	572.63	Joback Method
dvisc	0.0002599	Paxs	634.72	Joback Method

dvisc	0.0001666	Paxs	696.81	Joback Method
dvisc	0.0001149	Paxs	758.89	Joback Method
dvisc	0.0000838	Paxs	820.98	Joback Method
dvisc	0.0000639	Paxs	883.07	Joback Method
dvisc	0.0000505	Paxs	945.16	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339630&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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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