

Glutaric acid, cyclohexylmethyl 4-bromo-2-methoxyphenyl ester

Inchi:	InChI=1S/C19H25BrO5/c1-23-17-12-15(20)10-11-16(17)25-19(22)9-5-8-18(21)24-13-14
InchiKey:	NKHJBCUHKGIXIS-UHFFFAOYSA-N
Formula:	C19H25BrO5
SMILES:	COc1cc(Br)ccc1OC(=O)CCCC(=O)OCC1CCCCC1
Mol. weight [g/mol]:	413.30

Physical Properties

Property code	Value	Unit	Source
gf	-331.82	kJ/mol	Joback Method
hf	-763.07	kJ/mol	Joback Method
hfus	42.11	kJ/mol	Joback Method
hvap	89.07	kJ/mol	Joback Method
log10ws	-5.77		Crippen Method
logp	4.657		Crippen Method
mcvol	282.200	ml/mol	McGowan Method
pc	1747.74	kPa	Joback Method
rinqol	2873.00		NIST Webbook
tb	931.47	K	Joback Method
tc	1162.04	K	Joback Method
tf	589.08	K	Joback Method
vc	1.052	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	879.33	J/molxK	931.47	Joback Method
cpg	932.07	J/molxK	1123.62	Joback Method
cpg	924.63	J/molxK	1085.19	Joback Method
cpg	915.65	J/molxK	1046.76	Joback Method
cpg	905.12	J/molxK	1008.33	Joback Method
cpg	893.02	J/molxK	969.90	Joback Method
cpg	937.99	J/molxK	1162.04	Joback Method
dvisc	0.0000388	Paxs	931.47	Joback Method
dvisc	0.0000489	Paxs	874.40	Joback Method

dvisc	0.0000636	Paxs	817.34	Joback Method
dvisc	0.0000861	Paxs	760.27	Joback Method
dvisc	0.0001225	Paxs	703.21	Joback Method
dvisc	0.0001853	Paxs	646.14	Joback Method
dvisc	0.0003038	Paxs	589.08	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U393890&Units=SI

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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