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

Inchi: InChI=1S/C18H23BrO5/c1-22-16-11-14(19)7-8-15(16)24-18(21)10-9-17(20)23-12-13-5-3

InchiKey: KQEFSTWKYXEOPU-UHFFFAOYSA-N

Formula: C18H23BrO5

SMILES: COc1cc(Br)ccc1OC(=O)CCC(=O)OCC1CCCCC1

Mol. weight [g/mol]: 399.28

Physical Properties

Property code	Value	Unit	Source
gf	-340.24	kJ/mol	Joback Method
hf	-742.43	kJ/mol	Joback Method
hfus	39.52	kJ/mol	Joback Method
hvap	86.85	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	4.267		Crippen Method
mcvol	268.110	ml/mol	McGowan Method
pc	1896.95	kPa	Joback Method
rinpol	2804.00		NIST Webbook
rinpol	2804.00		NIST Webbook
tb	908.59	K	Joback Method
tc	1140.65	K	Joback Method
tf	577.81	K	Joback Method
vc	0.997	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	820.99	J/mol×K	908.59	Joback Method
cpg	834.77	J/mol×K	947.27	Joback Method
cpg	846.99	J/mol×K	985.94	Joback Method
cpg	857.66	J/mol×K	1024.62	Joback Method
cpg	866.80	J/mol×K	1063.29	Joback Method
cpg	874.42	J/mol×K	1101.97	Joback Method
cpg	880.54	J/mol×K	1140.65	Joback Method
dvisc	0.0003394	Pa×s	577.81	Joback Method

dvisc	0.0002094	Pa×s	632.94	Joback Method
dvisc	0.0001396	Pa×s	688.07	Joback Method
dvisc	0.0000988	Pa×s	743.20	Joback Method
dvisc	0.0000734	Pa×s	798.33	Joback Method
dvisc	0.0000566	Pa×s	853.46	Joback Method
dvisc	0.0000451	Pa×s	908.59	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=U390920&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