Succinic acid, di(5-bromo-2-methoxybenzyl) ester

Inchi: InChI=1S/C20H20Br2O6/c1-25-17-5-3-15(21)9-13(17)11-27-19(23)7-8-20(24)28-12-14-1

InchiKey: FYTWYJFPHCSPSQ-UHFFFAOYSA-N

Formula: C20H20Br2O6

SMILES: COc1ccc(Br)cc1COC(=O)CCC(=O)OCc1cc(Br)ccc1OC

Mol. weight [g/mol]: 516.18

Physical Properties

Property code	Value	Unit	Source
gf	-345.38	kJ/mol	Joback Method
hf	-730.33	kJ/mol	Joback Method
hfus	52.60	kJ/mol	Joback Method
hvap	103.32	kJ/mol	Joback Method
log10ws	-6.84		Crippen Method
logp	4.796		Crippen Method
mcvol	306.760	ml/mol	McGowan Method
pc	1826.28	kPa	Joback Method
rinpol	3371.00		NIST Webbook
rinpol	3371.00		NIST Webbook
tb	1060.02	K	Joback Method
tc	1306.50	K	Joback Method
tf	726.46	K	Joback Method
vc	1.147	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	886.15	J/mol×K	1060.02	Joback Method
cpg	893.71	J/mol×K	1101.10	Joback Method
cpg	899.62	J/mol×K	1142.18	Joback Method
cpg	903.89	J/mol×K	1183.26	Joback Method
cpg	906.50	J/mol×K	1224.34	Joback Method
cpg	907.48	J/mol×K	1265.42	Joback Method
cpg	906.82	J/mol×K	1306.50	Joback Method
dvisc	0.0000927	Pa×s	726.46	Joback Method

dvisc	0.0000651	Pa×s	782.05	Joback Method
dvisc	0.0000480	Pa×s	837.65	Joback Method
dvisc	0.0000367	Pa×s	893.24	Joback Method
dvisc	0.0000290	Pa×s	948.83	Joback Method
dvisc	0.0000235	Pa×s	1004.43	Joback Method
dvisc	0.0000194	Pa×s	1060.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381082&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

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