

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/molxK	1060.02	Joback Method
cpg	907.48	J/molxK	1265.42	Joback Method
cpg	906.50	J/molxK	1224.34	Joback Method
cpg	903.89	J/molxK	1183.26	Joback Method
cpg	899.62	J/molxK	1142.18	Joback Method
cpg	893.71	J/molxK	1101.10	Joback Method
cpg	906.82	J/molxK	1306.50	Joback Method
dvisc	0.0000194	Paxs	1060.02	Joback Method

dvisc	0.0000235	Paxs	1004.43	Joback Method
dvisc	0.0000290	Paxs	948.83	Joback Method
dvisc	0.0000367	Paxs	893.24	Joback Method
dvisc	0.0000480	Paxs	837.65	Joback Method
dvisc	0.0000651	Paxs	782.05	Joback Method
dvisc	0.0000927	Paxs	726.46	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

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