

Sebacic acid, ethyl 2-methoxy-5-bromobenzyl ester

Inchi:	InChI=1S/C20H29BrO5/c1-3-25-19(22)10-8-6-4-5-7-9-11-20(23)26-15-16-14-17(21)12-13
InchiKey:	JQQQCOMWXSKKRB-UHFFFAOYSA-N
Formula:	C20H29BrO5
SMILES:	CCOC(=O)CCCCCCCC(=O)OCc1cc(Br)ccc1OC
Mol. weight [g/mol]:	429.35

Physical Properties

Property code	Value	Unit	Source
gf	-347.85	kJ/mol	Joback Method
hf	-838.03	kJ/mol	Joback Method
hfus	52.87	kJ/mol	Joback Method
hvap	90.87	kJ/mol	Joback Method
log10ws	-6.38		Crippen Method
logp	5.185		Crippen Method
mvol	307.150	ml/mol	McGowan Method
pc	1378.88	kPa	Joback Method
rinpol	2893.00		NIST Webbook
rinpol	2893.00		NIST Webbook
tb	934.80	K	Joback Method
tc	1149.21	K	Joback Method
tf	592.97	K	Joback Method
vc	1.175	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	945.09	J/molxK	934.80	Joback Method
cpg	958.81	J/molxK	970.53	Joback Method
cpg	971.24	J/molxK	1006.27	Joback Method
cpg	982.40	J/molxK	1042.00	Joback Method
cpg	992.29	J/molxK	1077.74	Joback Method
cpg	1000.95	J/molxK	1113.47	Joback Method
cpg	1008.37	J/molxK	1149.21	Joback Method
dvisc	0.0002430	Paxs	592.97	Joback Method

dvisc	0.0001499	Paxs	649.94	Joback Method
dvisc	0.0000999	Paxs	706.91	Joback Method
dvisc	0.0000708	Paxs	763.88	Joback Method
dvisc	0.0000526	Paxs	820.86	Joback Method
dvisc	0.0000406	Paxs	877.83	Joback Method
dvisc	0.0000324	Paxs	934.80	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=U380640&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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