

Di-(p-bromophenacyl) succinate

Inchi:	InChI=1S/C20H16Br2O6/c21-15-5-1-13(2-6-15)17(23)11-27-19(25)9-10-20(26)28-12-18
InchiKey:	FNERLEDLNAIHAM-UHFFFAOYSA-N
Formula:	C20H16Br2O6
SMILES:	O=C(CCC(=O)OCC(=O)c1ccc(Br)cc1)OCC(=O)c1ccc(Br)cc1
Mol. weight [g/mol]:	512.14
CAS:	806-98-4

Physical Properties

Property code	Value	Unit	Source
gf	-373.96	kJ/mol	Joback Method
hf	-668.11	kJ/mol	Joback Method
hfus	54.20	kJ/mol	Joback Method
hvap	110.66	kJ/mol	Joback Method
log10ws	-6.17		Crippen Method
logp	4.144		Crippen Method
mcvol	298.160	ml/mol	McGowan Method
pc	2163.33	kPa	Joback Method
tb	1112.96	K	Joback Method
tc	1371.25	K	Joback Method
tf	756.82	K	Joback Method
vc	1.123	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	841.54	J/molxK	1112.96	Joback Method
cpg	861.38	J/molxK	1328.21	Joback Method
cpg	859.47	J/molxK	1285.16	Joback Method
cpg	856.60	J/molxK	1242.11	Joback Method
cpg	852.71	J/molxK	1199.06	Joback Method
cpg	847.71	J/molxK	1156.01	Joback Method
cpg	862.40	J/molxK	1371.25	Joback Method
dvisc	0.0000298	Paxs	1112.96	Joback Method
dvisc	0.0000364	Paxs	1053.60	Joback Method

dvisc	0.0000456	Paxs	994.25	Joback Method
dvisc	0.0000587	Paxs	934.89	Joback Method
dvisc	0.0000782	Paxs	875.53	Joback Method
dvisc	0.0001086	Paxs	816.18	Joback Method
dvisc	0.0001588	Paxs	756.82	Joback Method

Sources

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=C806984&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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