

Glutaric acid, di(4-bromobenzyl) ester

Inchi:	InChI=1S/C19H18Br2O4/c20-16-8-4-14(5-9-16)12-24-18(22)2-1-3-19(23)25-13-15-6-10-
InchiKey:	ZXQPAPWQOKEBBI-UHFFFAOYSA-N
Formula:	C19H18Br2O4
SMILES:	O=C(CCCC(=O)OCc1ccc(Br)cc1)OCc1ccc(Br)cc1
Mol. weight [g/mol]:	470.15

Physical Properties

Property code	Value	Unit	Source
gf	-124.54	kJ/mol	Joback Method
hf	-422.31	kJ/mol	Joback Method
hfus	48.41	kJ/mol	Joback Method
hvap	94.95	kJ/mol	Joback Method
log10ws	-7.02		Crippen Method
logp	5.169		Crippen Method
mcvol	280.930	ml/mol	McGowan Method
pc	2104.20	kPa	Joback Method
rinpola	3378.00		NIST Webbook
rinpola	3378.00		NIST Webbook
tb	982.34	K	Joback Method
tc	1227.67	K	Joback Method
tf	645.69	K	Joback Method
vc	1.056	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	785.03	J/molxK	982.34	Joback Method
cpg	795.29	J/molxK	1023.23	Joback Method
cpg	804.41	J/molxK	1064.12	Joback Method
cpg	812.46	J/molxK	1105.01	Joback Method
cpg	819.49	J/molxK	1145.89	Joback Method
cpg	825.58	J/molxK	1186.78	Joback Method
cpg	830.79	J/molxK	1227.67	Joback Method
dvisc	0.0002386	Paxs	645.69	Joback Method

dvisc	0.0001572	Paxs	701.80	Joback Method
dvisc	0.0001102	Paxs	757.91	Joback Method
dvisc	0.0000811	Paxs	814.02	Joback Method
dvisc	0.0000621	Paxs	870.12	Joback Method
dvisc	0.0000491	Paxs	926.23	Joback Method
dvisc	0.0000399	Paxs	982.34	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=U377535&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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