

Glutaric acid, 4-bromobenzyl butyl ester

Inchi:	InChI=1S/C16H21BrO4/c1-2-3-11-20-15(18)5-4-6-16(19)21-12-13-7-9-14(17)10-8-13/h7-
InchiKey:	RCHXIPFISRQRNV-UHFFFAOYSA-N
Formula:	C16H21BrO4
SMILES:	CCCCOC(=O)CCCC(=O)OCc1ccc(Br)cc1
Mol. weight [g/mol]:	357.24

Physical Properties

Property code	Value	Unit	Source
gf	-266.90	kJ/mol	Joback Method
hf	-611.78	kJ/mol	Joback Method
hfus	41.71	kJ/mol	Joback Method
hvap	78.90	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	4.006		Crippen Method
mvol	244.920	ml/mol	McGowan Method
pc	1928.74	kPa	Joback Method
rinpol	2574.00		NIST Webbook
rinpol	2574.00		NIST Webbook
tb	815.88	K	Joback Method
tc	1027.86	K	Joback Method
tf	513.14	K	Joback Method
vc	0.933	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	687.61	J/molxK	815.88	Joback Method
cpg	745.41	J/molxK	992.53	Joback Method
cpg	735.77	J/molxK	957.20	Joback Method
cpg	725.19	J/molxK	921.87	Joback Method
cpg	713.65	J/molxK	886.54	Joback Method
cpg	701.14	J/molxK	851.21	Joback Method
cpg	754.13	J/molxK	1027.86	Joback Method
dvisc	0.0000769	Paxs	815.88	Joback Method

dvisc	0.0000966	Paxs	765.42	Joback Method
dvisc	0.0001253	Paxs	714.97	Joback Method
dvisc	0.0001691	Paxs	664.51	Joback Method
dvisc	0.0002396	Paxs	614.05	Joback Method
dvisc	0.0003615	Paxs	563.60	Joback Method
dvisc	0.0005914	Paxs	513.14	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=U377531&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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