

Glutaric acid, 4-bromobenzyl isobutyl ester

Inchi:	InChI=1S/C16H21BrO4/c1-12(2)10-20-15(18)4-3-5-16(19)21-11-13-6-8-14(17)9-7-13/h6
InchiKey:	QPESDEWQBMIXOT-UHFFFAOYSA-N
Formula:	C16H21BrO4
SMILES:	CC(C)COC(=O)CCCC(=O)OCc1ccc(Br)cc1
Mol. weight [g/mol]:	357.24

Physical Properties

Property code	Value	Unit	Source
gf	-269.34	kJ/mol	Joback Method
hf	-617.06	kJ/mol	Joback Method
hfus	38.18	kJ/mol	Joback Method
hvap	78.51	kJ/mol	Joback Method
log10ws	-4.76		Crippen Method
logp	3.862		Crippen Method
mcvol	244.920	ml/mol	McGowan Method
pc	1942.37	kPa	Joback Method
rinpol	2523.00		NIST Webbook
rinpol	2523.00		NIST Webbook
tb	815.44	K	Joback Method
tc	1030.25	K	Joback Method
tf	498.14	K	Joback Method
vc	0.927	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	688.18	J/molxK	815.44	Joback Method
cpg	701.88	J/molxK	851.24	Joback Method
cpg	714.53	J/molxK	887.04	Joback Method
cpg	726.16	J/molxK	922.85	Joback Method
cpg	736.79	J/molxK	958.65	Joback Method
cpg	746.45	J/molxK	994.45	Joback Method
cpg	755.17	J/molxK	1030.25	Joback Method
dvisc	0.0006585	Paxs	498.14	Joback Method

dvisc	0.0003796	Paxs	551.02	Joback Method
dvisc	0.0002410	Paxs	603.91	Joback Method
dvisc	0.0001647	Paxs	656.79	Joback Method
dvisc	0.0001191	Paxs	709.67	Joback Method
dvisc	0.0000900	Paxs	762.56	Joback Method
dvisc	0.0000706	Paxs	815.44	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=U377530&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
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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