

Glutaric acid, 3-bromobenzyl ethyl ester

Inchi:	InChI=1S/C14H17BrO4/c1-2-18-13(16)7-4-8-14(17)19-10-11-5-3-6-12(15)9-11/h3,5-6,9H
InchiKey:	CBJAGKUCPMOZHL-UHFFFAOYSA-N
Formula:	C14H17BrO4
SMILES:	CCOC(=O)CCCC(=O)OCc1cccc(Br)c1
Mol. weight [g/mol]:	329.19

Physical Properties

Property code	Value	Unit	Source
gf	-283.74	kJ/mol	Joback Method
hf	-570.50	kJ/mol	Joback Method
hfus	36.53	kJ/mol	Joback Method
hvap	74.44	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	3.226		Crippen Method
mcvol	216.740	ml/mol	McGowan Method
pc	2300.32	kPa	Joback Method
rinpol	2404.00		NIST Webbook
rinpol	2404.00		NIST Webbook
tb	770.12	K	Joback Method
tc	986.25	K	Joback Method
tf	490.60	K	Joback Method
vc	0.822	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	577.72	J/molxK	770.12	Joback Method
cpg	590.59	J/molxK	806.14	Joback Method
cpg	602.53	J/molxK	842.16	Joback Method
cpg	613.53	J/molxK	878.18	Joback Method
cpg	623.64	J/molxK	914.21	Joback Method
cpg	632.85	J/molxK	950.23	Joback Method
cpg	641.19	J/molxK	986.25	Joback Method
dvisc	0.0007115	Paxs	490.60	Joback Method

dvisc	0.0004468	Paxs	537.19	Joback Method
dvisc	0.0003022	Paxs	583.77	Joback Method
dvisc	0.0002166	Paxs	630.36	Joback Method
dvisc	0.0001625	Paxs	676.95	Joback Method
dvisc	0.0001265	Paxs	723.53	Joback Method
dvisc	0.0001015	Paxs	770.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377676&Units=SI
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

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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