

Glutaric acid, 3-methylbut-2-yl 4-bromophenyl ester

Inchi:	InChI=1S/C16H21BrO4/c1-11(2)12(3)20-15(18)5-4-6-16(19)21-14-9-7-13(17)8-10-14/h7
InchiKey:	FFVHPRGSXORMDM-UHFFFAOYSA-N
Formula:	C16H21BrO4
SMILES:	CC(C)C(C)OC(=O)CCCC(=O)Oc1ccc(Br)cc1
Mol. weight [g/mol]:	357.24

Physical Properties

Property code	Value	Unit	Source
gf	-271.78	kJ/mol	Joback Method
hf	-622.34	kJ/mol	Joback Method
hfus	34.66	kJ/mol	Joback Method
hvap	78.12	kJ/mol	Joback Method
log10ws	-5.03		Crippen Method
logp	4.112		Crippen Method
mcvol	244.920	ml/mol	McGowan Method
pc	1956.14	kPa	Joback Method
rinpol	2282.00		NIST Webbook
rinpol	2282.00		NIST Webbook
tb	815.00	K	Joback Method
tc	1032.80	K	Joback Method
tf	483.14	K	Joback Method
vc	0.921	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	688.76	J/molxK	815.00	Joback Method
cpg	702.63	J/molxK	851.30	Joback Method
cpg	715.42	J/molxK	887.60	Joback Method
cpg	727.15	J/molxK	923.90	Joback Method
cpg	737.84	J/molxK	960.20	Joback Method
cpg	747.52	J/molxK	996.50	Joback Method
cpg	756.22	J/molxK	1032.80	Joback Method
dvisc	0.0007442	Paxs	483.14	Joback Method

dvisc	0.0004021	Paxs	538.45	Joback Method
dvisc	0.0002436	Paxs	593.76	Joback Method
dvisc	0.0001608	Paxs	649.07	Joback Method
dvisc	0.0001132	Paxs	704.38	Joback Method
dvisc	0.0000839	Paxs	759.69	Joback Method
dvisc	0.0000648	Paxs	815.00	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=U393286&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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