Glutaric acid, 3-methylbut-2-en-1-yl 4-bromophenyl ester

Inchi: InChI=1S/C16H19BrO4/c1-12(2)10-11-20-15(18)4-3-5-16(19)21-14-8-6-13(17)7-9-14/h6-

InchiKey: KCMDEFRQPOZZSB-UHFFFAOYSA-N

Formula: C16H19BrO4

SMILES: CC(C)=CCOC(=O)CCCC(=O)Oc1ccc(Br)cc1

Mol. weight [g/mol]: 355.22

Physical Properties

Property code	Value	Unit	Source
gf	-195.23	kJ/mol	Joback Method
hf	-504.35	kJ/mol	Joback Method
hfus	40.60	kJ/mol	Joback Method
hvap	78.93	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	4.034		Crippen Method
mcvol	240.620	ml/mol	McGowan Method
pc	2029.06	kPa	Joback Method
rinpol	2392.00		NIST Webbook
rinpol	2392.00		NIST Webbook
tb	819.92	K	Joback Method
tc	1040.54	K	Joback Method
tf	494.10	K	Joback Method
vc	0.914	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	660.91	J/mol×K	819.92	Joback Method
cpg	674.08	J/mol×K	856.69	Joback Method
cpg	686.27	J/mol×K	893.46	Joback Method
cpg	697.54	J/mol×K	930.23	Joback Method
cpg	707.90	J/mol×K	967.00	Joback Method
cpg	717.41	J/mol×K	1003.77	Joback Method
cpg	726.11	J/mol×K	1040.54	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=U393288&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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