Glutaric acid, 2-ethylhexyl 4-bromo-2-methoxyphenyl ester

Inchi: InChI=1S/C20H29BrO5/c1-4-6-8-15(5-2)14-25-19(22)9-7-10-20(23)26-17-12-11-16(21)13

InchiKey: CYHKZMSECOXDBB-UHFFFAOYSA-N

Formula: C20H29BrO5

SMILES: CCCCC(CC)COC(=O)CCCC(=O)Oc1ccc(Br)cc1OC

Mol. weight [g/mol]: 429.35

Physical Properties

Property code	Value	Unit	Source
gf	-350.29	kJ/mol	Joback Method
hf	-843.31	kJ/mol	Joback Method
hfus	49.34	kJ/mol	Joback Method
hvap	90.48	kJ/mol	Joback Method
log10ws	-6.29		Crippen Method
logp	5.293		Crippen Method
mcvol	307.150	ml/mol	McGowan Method
pc	1387.11	kPa	Joback Method
rinpol	2766.00		NIST Webbook
rinpol	2766.00		NIST Webbook
tb	934.36	K	Joback Method
tc	1149.94	K	Joback Method
tf	577.97	K	Joback Method
vc	1.169	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	945.56	J/mol×K	934.36	Joback Method
cpg	959.31	J/mol×K	970.29	Joback Method
cpg	971.75	J/mol×K	1006.22	Joback Method
cpg	982.89	J/mol×K	1042.15	Joback Method
cpg	992.74	J/mol×K	1078.08	Joback Method
cpg	1001.32	J/mol×K	1114.01	Joback Method
cpg	1008.64	J/mol×K	1149.94	Joback Method
dvisc	0.0002618	Pa×s	577.97	Joback Method

dvisc	0.0001536	Pa×s	637.37	Joback Method
dvisc	0.0000987	Pa×s	696.77	Joback Method
dvisc	0.0000680	Pa×s	756.16	Joback Method
dvisc	0.0000495	Pa×s	815.56	Joback Method
dvisc	0.0000376	Pa×s	874.96	Joback Method
dvisc	0.0000295	Pa×s	934.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393889&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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