Glutaric acid, dec-2-yl 4-bromo-2-methoxyphenyl ester

Inchi: InChI=1S/C22H33BrO5/c1-4-5-6-7-8-9-11-17(2)27-21(24)12-10-13-22(25)28-19-15-14-18

InchiKey: WNMLUGRWOIXZDU-UHFFFAOYSA-N

Formula: C22H33BrO5

SMILES: CCCCCCCCC(C)OC(=O)CCCC(=O)Oc1ccc(Br)cc1OC

Mol. weight [g/mol]: 457.40

Physical Properties

Property code	Value	Unit	Source
gf	-333.45	kJ/mol	Joback Method
hf	-884.59	kJ/mol	Joback Method
hfus	54.52	kJ/mol	Joback Method
hvap	94.93	kJ/mol	Joback Method
log10ws	-7.48		Crippen Method
logp	6.216		Crippen Method
mcvol	335.330	ml/mol	McGowan Method
pc	1208.15	kPa	Joback Method
rinpol	2930.00		NIST Webbook
rinpol	2930.00		NIST Webbook
tb	980.12	K	Joback Method
tc	1201.06	K	Joback Method
tf	600.51	K	Joback Method
vc	1.282	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1065.14	J/mol×K	980.12	Joback Method
cpg	1079.12	J/mol×K	1016.94	Joback Method
cpg	1091.64	J/mol×K	1053.77	Joback Method
cpg	1102.73	J/mol×K	1090.59	Joback Method
cpg	1112.40	J/mol×K	1127.41	Joback Method
cpg	1120.69	J/mol×K	1164.24	Joback Method
cpg	1127.60	J/mol×K	1201.06	Joback Method
dvisc	0.0002068	Pa×s	600.51	Joback Method

dvisc	0.0001188	Pa×s	663.78	Joback Method
dvisc	0.0000751	Pa×s	727.05	Joback Method
dvisc	0.0000511	Pa×s	790.31	Joback Method
dvisc	0.0000368	Pa×s	853.58	Joback Method
dvisc	0.0000278	Pa×s	916.85	Joback Method
dvisc	0.0000217	Pa×s	980.12	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=U393893&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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