Glutaric acid, dodec-2-en-1-yl 4-bromophenyl ester

Inchi: InChI=1S/C23H33BrO4/c1-2-3-4-5-6-7-8-9-10-11-19-27-22(25)13-12-14-23(26)28-21-17-

InchiKey: XDBDHUVFSBDYIO-ZHACJKMWSA-N

Formula: C23H33BrO4

SMILES: CCCCCCCCCC=CCOC(=O)CCCC(=O)Oc1ccc(Br)cc1

Mol. weight [g/mol]: 453.41

Physical Properties

Property code	Value	Unit	Source
gf	-127.74	kJ/mol	Joback Method
hf	-639.04	kJ/mol	Joback Method
hfus	60.04	kJ/mol	Joback Method
hvap	94.44	kJ/mol	Joback Method
log10ws	-7.94		Crippen Method
logp	6.765		Crippen Method
mcvol	339.250	ml/mol	McGowan Method
pc	1191.52	kPa	Joback Method
rinpol	3117.00		NIST Webbook
rinpol	3117.00		NIST Webbook
tb	980.20	K	Joback Method
tc	1201.50	K	Joback Method
tf	586.95	K	Joback Method
vc	1.306	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1069.74	J/mol×K	980.20	Joback Method
cpg	1133.24	J/mol×K	1164.62	Joback Method
cpg	1122.59	J/mol×K	1127.73	Joback Method
cpg	1110.99	J/mol×K	1090.85	Joback Method
cpg	1098.35	J/mol×K	1053.97	Joback Method
cpg	1084.63	J/mol×K	1017.08	Joback Method
cpg	1142.98	J/mol×K	1201.50	Joback Method
dvisc	0.0000238	Pa×s	980.20	Joback Method

dvisc	0.0000307	Pa×s	914.66	Joback Method
dvisc	0.0000411	Pa×s	849.12	Joback Method
dvisc	0.0000577	Pa×s	783.58	Joback Method
dvisc	0.0000863	Pa×s	718.03	Joback Method
dvisc	0.0001400	Pa×s	652.49	Joback Method
dvisc	0.0002529	Pa×s	586.95	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393299&Units=SI

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