Glutaric acid, dodec-2-en-1-yl 4-bromo-2-methoxyphenyl ester

Inchi: InChI=1S/C24H35BrO5/c1-3-4-5-6-7-8-9-10-11-12-18-29-23(26)14-13-15-24(27)30-21-1

InchiKey: CXNUODQXYPWUCZ-VAWYXSNFSA-N

Formula: C24H35BrO5

SMILES: CCCCCCCCCC=CCOC(=O)CCCC(=O)Oc1ccc(Br)cc1OC

Mol. weight [g/mol]: 483.44

Physical Properties

Property code	Value	Unit	Source
gf	-233.95	kJ/mol	Joback Method
hf	-803.37	kJ/mol	Joback Method
hfus	63.43	kJ/mol	Joback Method
hvap	99.73	kJ/mol	Joback Method
log10ws	-8.06		Crippen Method
logp	6.773		Crippen Method
mcvol	359.210	ml/mol	McGowan Method
pc	1092.82	kPa	Joback Method
rinpol	3249.00		NIST Webbook
tb	1030.48	K	Joback Method
tc	1261.64	K	Joback Method
tf	632.97	K	Joback Method
vc	1.379	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1157.21	J/mol×K	1030.48	Joback Method
cpg	1171.40	J/mol×K	1069.01	Joback Method
cpg	1184.15	J/mol×K	1107.53	Joback Method
cpg	1195.50	J/mol×K	1146.06	Joback Method
cpg	1205.52	J/mol×K	1184.59	Joback Method
cpg	1214.25	J/mol×K	1223.12	Joback Method
cpg	1221.74	J/mol×K	1261.64	Joback Method
dvisc	0.0001396	Pa×s	632.97	Joback Method
dvisc	0.0000812	Pa×s	699.22	Joback Method

dvisc	0.0000519	Pa×s	765.47	Joback Method
dvisc	0.0000356	Pa×s	831.73	Joback Method
dvisc	0.0000258	Pa×s	897.98	Joback Method
dvisc	0.0000196	Pa×s	964.23	Joback Method
dvisc	0.0000154	Pa×s	1030.48	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=U393895&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

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