

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:	CCCCCCCCC=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
rinqol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0000519	Paxs	765.47	Joback Method
dvisc	0.0000356	Paxs	831.73	Joback Method
dvisc	0.0000258	Paxs	897.98	Joback Method
dvisc	0.0000196	Paxs	964.23	Joback Method
dvisc	0.0000154	Paxs	1030.48	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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