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

Inchi: InChI=1S/C23H33BrO5/c1-3-4-5-6-7-8-9-10-11-12-17-28-22(25)15-16-23(26)29-20-14-13

InchiKey: XGGYOPFFKQJDQZ-VAWYXSNFSA-N

Formula: C23H33BrO5

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

Mol. weight [g/mol]: 469.41

Physical Properties

Property code	Value	Unit	Source
gf	-242.37	kJ/mol	Joback Method
hf	-782.73	kJ/mol	Joback Method
hfus	60.84	kJ/mol	Joback Method
hvap	97.51	kJ/mol	Joback Method
log10ws	-7.64		Crippen Method
logp	6.383		Crippen Method
mcvol	345.120	ml/mol	McGowan Method
pc	1165.63	kPa	Joback Method
rinpol	3192.00		NIST Webbook
rinpol	3192.00		NIST Webbook
tb	1007.60	K	Joback Method
tc	1233.86	K	Joback Method
tf	621.70	K	Joback Method
vc	1.323	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1096.33	J/mol×K	1007.60	Joback Method
cpg	1153.01	J/mol×K	1196.15	Joback Method
cpg	1144.22	J/mol×K	1158.44	Joback Method
cpg	1134.20	J/mol×K	1120.73	Joback Method
cpg	1122.91	J/mol×K	1083.02	Joback Method
cpg	1110.30	J/mol×K	1045.31	Joback Method
cpg	1160.62	J/mol×K	1233.86	Joback Method
dvisc	0.0000180	Pa×s	1007.60	Joback Method

dvisc	0.0000228	Pa×s	943.28	Joback Method
dvisc	0.0000300	Pa×s	878.97	Joback Method
dvisc	0.0000411	Pa×s	814.65	Joback Method
dvisc	0.0000596	Pa×s	750.33	Joback Method
dvisc	0.0000926	Pa×s	686.02	Joback Method
dvisc	0.0001577	Pa×s	621.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390926&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