Diethylmalonic acid, 4-bromo-2-methoxyphenyl undecyl ester

Inchi: InChI=1S/C25H39BrO5/c1-5-8-9-10-11-12-13-14-15-18-30-23(27)25(6-2,7-3)24(28)31-21

InchiKey: HDEUNJPWVYRILL-UHFFFAOYSA-N

Formula: C25H39BrO5

SMILES: CCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(Br)cc1OC

Mol. weight [g/mol]: 499.48

Physical Properties

Property code	Value	Unit	Source
gf	-302.91	kJ/mol	Joback Method
hf	-949.98	kJ/mol	Joback Method
hfus	58.40	kJ/mol	Joback Method
hvap	100.70	kJ/mol	Joback Method
log10ws	-8.39		Crippen Method
logp	7.244		Crippen Method
mcvol	377.600	ml/mol	McGowan Method
pc	1005.26	kPa	Joback Method
rinpol	3034.00		NIST Webbook
rinpol	3034.00		NIST Webbook
tb	1045.97	K	Joback Method
tc	1280.89	K	Joback Method
tf	651.74	K	Joback Method
vc	1.444	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1247.83	J/mol×K	1045.97	Joback Method
cpg	1262.47	J/mol×K	1085.12	Joback Method
cpg	1275.58	J/mol×K	1124.28	Joback Method
cpg	1287.22	J/mol×K	1163.43	Joback Method
cpg	1297.45	J/mol×K	1202.59	Joback Method
cpg	1306.34	J/mol×K	1241.74	Joback Method
cpg	1313.96	J/mol×K	1280.89	Joback Method
dvisc	0.0001110	Pa×s	651.74	Joback Method

dvisc	0.0000635	Pa×s	717.45	Joback Method
dvisc	0.0000399	Pa×s	783.15	Joback Method
dvisc	0.0000269	Pa×s	848.86	Joback Method
dvisc	0.0000192	Pa×s	914.56	Joback Method
dvisc	0.0000143	Pa×s	980.26	Joback Method
dvisc	0.0000111	Pa×s	1045.97	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=U371162&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