Diethylmalonic acid, dodecyl 4-fluoro-2-methoxyphenyl ester

Inchi: InChI=1S/C26H41FO5/c1-5-8-9-10-11-12-13-14-15-16-19-31-24(28)26(6-2,7-3)25(29)32

InchiKey: BLLXRVMTUQFLRC-UHFFFAOYSA-N

Formula: C26H41FO5

SMILES: CCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(F)cc1OC

Mol. weight [g/mol]: 452.60

Physical Properties

Property code	Value	Unit	Source
gf	-503.62	kJ/mol	Joback Method
hf	-1193.06	kJ/mol	Joback Method
hfus	58.79	kJ/mol	Joback Method
hvap	95.68	kJ/mol	Joback Method
log10ws	-7.97		Crippen Method
logp	7.010		Crippen Method
mcvol	375.960	ml/mol	McGowan Method
pc	883.67	kPa	Joback Method
rinpol	2856.00		NIST Webbook
tb	1001.96	K	Joback Method
tc	1228.15	K	Joback Method
tf	603.80	K	Joback Method
vc	1.456	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1279.07	J/mol×K	1001.96	Joback Method
cpg	1295.62	J/mol×K	1039.66	Joback Method
cpg	1310.53	J/mol×K	1077.36	Joback Method
cpg	1323.85	J/mol×K	1115.06	Joback Method
cpg	1335.63	J/mol×K	1152.76	Joback Method
cpg	1345.92	J/mol×K	1190.45	Joback Method
cpg	1354.80	J/mol×K	1228.15	Joback Method

Sources

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=U370889&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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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