Diethylmalonic acid, 2-formylphenyl octyl ester

Inchi: InChI=1S/C22H32O5/c1-4-7-8-9-10-13-16-26-20(24)22(5-2,6-3)21(25)27-19-15-12-11-14

InchiKey: ICJISCSIRIDCBK-UHFFFAOYSA-N

Formula: C22H32O5

SMILES: CCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccccc1C=O

Mol. weight [g/mol]: 376.49

Physical Properties

Property code	Value	Unit	Source
gf	-327.38	kJ/mol	Joback Method
hf	-856.28	kJ/mol	Joback Method
hfus	46.84	kJ/mol	Joback Method
hvap	91.24	kJ/mol	Joback Method
log10ws	-6.09		Crippen Method
logp	5.115		Crippen Method
mcvol	313.530	ml/mol	McGowan Method
pc	1249.49	kPa	Joback Method
rinpol	2551.00		NIST Webbook
tb	932.43	K	Joback Method
tc	1145.72	K	Joback Method
tf	565.38	K	Joback Method
vc	1.214	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1013.00	J/mol×K	932.43	Joback Method
cpg	1027.78	J/mol×K	967.98	Joback Method
cpg	1041.34	J/mol×K	1003.53	Joback Method
cpg	1053.74	J/mol×K	1039.08	Joback Method
cpg	1065.03	J/mol×K	1074.62	Joback Method
cpg	1075.26	J/mol×K	1110.17	Joback Method
cpg	1084.48	J/mol×K	1145.72	Joback Method
dvisc	0.0003973	Pa×s	565.38	Joback Method
dvisc	0.0002158	Pa×s	626.55	Joback Method

dvisc	0.0001307	Pa×s	687.73	Joback Method
dvisc	0.0000859	Pa×s	748.90	Joback Method
dvisc	0.0000601	Pa×s	810.08	Joback Method
dvisc	0.0000443	Pa×s	871.25	Joback Method
dvisc	0.0000339	Pa×s	932.43	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=U369953&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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