Diethylmalonic acid, 2-formylphenyl heptyl ester

Inchi: InChI=1S/C21H30O5/c1-4-7-8-9-12-15-25-19(23)21(5-2,6-3)20(24)26-18-14-11-10-13-17

InchiKey: LYCMPLCWVDESBM-UHFFFAOYSA-N

Formula: C21H30O5

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

Mol. weight [g/mol]: 362.46

Physical Properties

Property code	Value	Unit	Source
gf	-335.80	kJ/mol	Joback Method
hf	-835.64	kJ/mol	Joback Method
hfus	44.25	kJ/mol	Joback Method
hvap	89.01	kJ/mol	Joback Method
log10ws	-5.67		Crippen Method
logp	4.724		Crippen Method
mcvol	299.440	ml/mol	McGowan Method
pc	1338.82	kPa	Joback Method
rinpol	2450.00		NIST Webbook
rinpol	2450.00		NIST Webbook
tb	909.55	K	Joback Method
tc	1120.94	K	Joback Method
tf	554.11	K	Joback Method
vc	1.157	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	953.37	J/mol×K	909.55	Joback Method
cpg	967.95	J/mol×K	944.78	Joback Method
cpg	981.36	J/mol×K	980.01	Joback Method
cpg	993.63	J/mol×K	1015.24	Joback Method
cpg	1004.83	J/mol×K	1050.48	Joback Method
cpg	1014.99	J/mol×K	1085.71	Joback Method
cpg	1024.17	J/mol×K	1120.94	Joback Method
dvisc	0.0004472	Pa×s	554.11	Joback Method

dvisc	0.0002455	Pa×s	613.35	Joback Method
dvisc	0.0001498	Pa×s	672.59	Joback Method
dvisc	0.0000990	Pa×s	731.83	Joback Method
dvisc	0.0000697	Pa×s	791.07	Joback Method
dvisc	0.0000515	Pa×s	850.31	Joback Method
dvisc	0.0000395	Pa×s	909.55	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=U369952&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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