

Diethylmalonic acid, heptyl 2-nitrophenyl ester

Inchi:	InChI=1S/C20H29NO6/c1-4-7-8-9-12-15-26-18(22)20(5-2,6-3)19(23)27-17-14-11-10-13-
InchiKey:	QJHGIGRMZLBGAZ-UHFFFAOYSA-N
Formula:	C20H29NO6
SMILES:	CCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cccc1[N+](=O)[O-]
Mol. weight [g/mol]:	379.45

Physical Properties

Property code	Value	Unit	Source
gf	-209.15	kJ/mol	Joback Method
hf	-740.18	kJ/mol	Joback Method
hfus	50.73	kJ/mol	Joback Method
hvap	96.66	kJ/mol	Joback Method
log10ws	-6.08		Crippen Method
logp	4.820		Crippen Method
mvol	301.200	ml/mol	McGowan Method
pc	1372.76	kPa	Joback Method
rinpol	2552.00		NIST Webbook
rinpol	2552.00		NIST Webbook
tb	989.85	K	Joback Method
tc	1218.67	K	Joback Method
tf	644.45	K	Joback Method
vc	1.167	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	988.78	J/molxK	989.85	Joback Method
cpg	1001.61	J/molxK	1027.99	Joback Method
cpg	1013.19	J/molxK	1066.12	Joback Method
cpg	1023.58	J/molxK	1104.26	Joback Method
cpg	1032.86	J/molxK	1142.40	Joback Method
cpg	1041.08	J/molxK	1180.54	Joback Method
cpg	1048.30	J/molxK	1218.67	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U369861&Units=SI

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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