

Diethylmalonic acid, dodecyl 3-methylpent-2-yl ester

Inchi:	InChI=1S/C25H48O4/c1-7-11-12-13-14-15-16-17-18-19-20-28-23(26)25(9-3,10-4)24(27)
InchiKey:	AJMXQDZCIUMAIN-UHFFFAOYSA-N
Formula:	C25H48O4
SMILES:	CCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OC(C)C(C)CC
Mol. weight [g/mol]:	412.65

Physical Properties

Property code	Value	Unit	Source
gf	-310.26	kJ/mol	Joback Method
hf	-1068.24	kJ/mol	Joback Method
hfus	51.62	kJ/mol	Joback Method
hvap	87.48	kJ/mol	Joback Method
log10ws	-7.64		Crippen Method
logp	7.235		Crippen Method
mcvol	377.990	ml/mol	McGowan Method
pc	820.54	kPa	Joback Method
rinpol	2470.00		NIST Webbook
tb	919.87	K	Joback Method
tc	1126.52	K	Joback Method
tf	488.25	K	Joback Method
vc	1.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1281.85	J/molxK	919.87	Joback Method
cpg	1302.06	J/molxK	954.31	Joback Method
cpg	1320.85	J/molxK	988.75	Joback Method
cpg	1338.27	J/molxK	1023.20	Joback Method
cpg	1354.40	J/molxK	1057.64	Joback Method
cpg	1369.27	J/molxK	1092.08	Joback Method
cpg	1382.95	J/molxK	1126.52	Joback Method
dvisc	0.0005773	Paxs	488.25	Joback Method
dvisc	0.0002172	Paxs	560.19	Joback Method

dvisc	0.0001021	Paxs	632.12	Joback Method
dvisc	0.0000560	Paxs	704.06	Joback Method
dvisc	0.0000343	Paxs	776.00	Joback Method
dvisc	0.0000228	Paxs	847.93	Joback Method
dvisc	0.0000162	Paxs	919.87	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369737&Units=SI
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

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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