

Diethylmalonic acid, 4-chlorobenzyl dodecyl ester

Inchi:	InChI=1S/C26H41ClO4/c1-4-7-8-9-10-11-12-13-14-15-20-30-24(28)26(5-2,6-3)25(29)31-
InchiKey:	IVVMUBQURSKRIC-UHFFFAOYSA-N
Formula:	C26H41ClO4
SMILES:	CCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCc1ccc(Cl)cc1
Mol. weight [g/mol]:	453.05

Physical Properties

Property code	Value	Unit	Source
gf	-206.11	kJ/mol	Joback Method
hf	-869.00	kJ/mol	Joback Method
hfus	59.10	kJ/mol	Joback Method
hvap	97.81	kJ/mol	Joback Method
log10ws	-8.47		Crippen Method
logp	7.654		Crippen Method
mvol	380.560	ml/mol	McGowan Method
pc	905.06	kPa	Joback Method
rinpol	2981.00		NIST Webbook
rinpol	2981.00		NIST Webbook
tb	1012.72	K	Joback Method
tc	1240.09	K	Joback Method
tf	598.38	K	Joback Method
vc	1.470	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1269.75	J/molxK	1012.72	Joback Method
cpg	1286.19	J/molxK	1050.62	Joback Method
cpg	1301.21	J/molxK	1088.51	Joback Method
cpg	1314.90	J/molxK	1126.41	Joback Method
cpg	1327.34	J/molxK	1164.30	Joback Method
cpg	1338.60	J/molxK	1202.20	Joback Method
cpg	1348.78	J/molxK	1240.09	Joback Method
dvisc	0.0002050	Paxs	598.38	Joback Method

dvisc	0.0001046	Paxs	667.44	Joback Method
dvisc	0.0000606	Paxs	736.49	Joback Method
dvisc	0.0000385	Paxs	805.55	Joback Method
dvisc	0.0000263	Paxs	874.61	Joback Method
dvisc	0.0000190	Paxs	943.66	Joback Method
dvisc	0.0000144	Paxs	1012.72	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369784&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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