

Diethylmalonic acid, 2-ethoxyethyl octyl ester

Inchi:	InChI=1S/C19H36O5/c1-5-9-10-11-12-13-14-23-17(20)19(6-2,7-3)18(21)24-16-15-22-8-4
InchiKey:	KAWHNQXDZCSHST-UHFFFAOYSA-N
Formula:	C19H36O5
SMILES:	CCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCOCC
Mol. weight [g/mol]:	344.49

Physical Properties

Property code	Value	Unit	Source
gf	-460.90	kJ/mol	Joback Method
hf	-1066.06	kJ/mol	Joback Method
hfus	44.31	kJ/mol	Joback Method
hvap	77.31	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	4.276		Crippen Method
mcvol	299.320	ml/mol	McGowan Method
pc	1150.65	kPa	Joback Method
rinsol	2034.00		NIST Webbook
tb	805.89	K	Joback Method
tc	991.96	K	Joback Method
tf	472.86	K	Joback Method
vc	1.155	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	941.33	J/molxK	805.89	Joback Method
cpg	958.94	J/molxK	836.90	Joback Method
cpg	975.48	J/molxK	867.91	Joback Method
cpg	990.99	J/molxK	898.92	Joback Method
cpg	1005.48	J/molxK	929.94	Joback Method
cpg	1018.97	J/molxK	960.95	Joback Method
cpg	1031.48	J/molxK	991.96	Joback Method
dvisc	0.0006049	Paxs	472.86	Joback Method
dvisc	0.0002972	Paxs	528.37	Joback Method

dvisc	0.0001672	Paxs	583.87	Joback Method
dvisc	0.0001039	Paxs	639.38	Joback Method
dvisc	0.0000697	Paxs	694.88	Joback Method
dvisc	0.0000496	Paxs	750.38	Joback Method
dvisc	0.0000370	Paxs	805.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370610&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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