

2-Ethylhexyl nonadecanoate

Inchi:	InChI=1S/C27H54O2/c1-4-7-9-10-11-12-13-14-15-16-17-18-19-20-21-22-24-27(28)29-25
InchiKey:	BIKNLYWCEZZIGI-UHFFFAOYSA-N
Formula:	C27H54O2
SMILES:	CCCCCCCCCCCCCCCCCCC(=O)OCC(CC)CCCC
Mol. weight [g/mol]:	410.72

Physical Properties

Property code	Value	Unit	Source
gf	-59.90	kJ/mol	Joback Method
hf	-850.69	kJ/mol	Joback Method
hfus	64.95	kJ/mol	Joback Method
hvap	84.46	kJ/mol	Joback Method
log10ws	-9.75		Crippen Method
logp	9.398		Crippen Method
mcvol	398.730	ml/mol	McGowan Method
pc	708.84	kPa	Joback Method
rinpola	2775.00		NIST Webbook
rinpola	2775.00		NIST Webbook
tb	893.01	K	Joback Method
tc	1096.23	K	Joback Method
tf	451.21	K	Joback Method
vc	1.565	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1350.92	J/molxK	893.01	Joback Method
cpg	1374.45	J/molxK	926.88	Joback Method
cpg	1396.52	J/molxK	960.75	Joback Method
cpg	1417.19	J/molxK	994.62	Joback Method
cpg	1436.51	J/molxK	1028.49	Joback Method
cpg	1454.55	J/molxK	1062.36	Joback Method
cpg	1471.36	J/molxK	1096.23	Joback Method
dvisc	0.0008713	Paxs	451.21	Joback Method

dvisc	0.0003163	Paxs	524.84	Joback Method
dvisc	0.0001473	Paxs	598.48	Joback Method
dvisc	0.0000811	Paxs	672.11	Joback Method
dvisc	0.0000503	Paxs	745.74	Joback Method
dvisc	0.0000339	Paxs	819.38	Joback Method
dvisc	0.0000245	Paxs	893.01	Joback Method

Sources

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=R540415&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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