

decyl heptadecanoate

Inchi:	InChI=1S/C27H54O2/c1-3-5-7-9-11-13-14-15-16-17-18-19-21-23-25-27(28)29-26-24-22-
InchiKey:	UFNTWTLRQBICFA-UHFFFAOYSA-N
Formula:	C27H54O2
SMILES:	CCCCCCCCCCCCCCCC(=O)CCCCCCCC
Mol. weight [g/mol]:	410.72

Physical Properties

Property code	Value	Unit	Source
gf	-57.46	kJ/mol	Joback Method
hf	-845.41	kJ/mol	Joback Method
hfus	68.47	kJ/mol	Joback Method
hvap	84.85	kJ/mol	Joback Method
log10ws	-9.99		Crippen Method
logp	9.542		Crippen Method
mvol	398.730	ml/mol	McGowan Method
pc	705.83	kPa	Joback Method
rinpol	2854.03		NIST Webbook
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tb	893.45	K	Joback Method
tc	1097.77	K	Joback Method
tf	466.21	K	Joback Method
vc	1.571	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1350.54	J/molxK	893.45	Joback Method
cpg	1374.21	J/molxK	927.50	Joback Method
cpg	1396.42	J/molxK	961.56	Joback Method
cpg	1417.22	J/molxK	995.61	Joback Method
cpg	1436.68	J/molxK	1029.66	Joback Method
cpg	1454.85	J/molxK	1063.71	Joback Method
cpg	1471.80	J/molxK	1097.77	Joback Method
dvisc	0.0007281	Paxs	466.21	Joback Method

dvisc	0.0002915	Paxs	537.42	Joback Method
dvisc	0.0001446	Paxs	608.62	Joback Method
dvisc	0.0000831	Paxs	679.83	Joback Method
dvisc	0.0000530	Paxs	751.04	Joback Method
dvisc	0.0000366	Paxs	822.24	Joback Method
dvisc	0.0000268	Paxs	893.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R437502&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

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
pc:	Critical Pressure
rin_{pol}:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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