

Fumaric acid, dec-4-enyl pentadecyl ester

Inchi:	InChI=1S/C29H52O4/c1-3-5-7-9-11-13-14-15-16-17-19-21-23-27-33-29(31)25-24-28(30)
InchiKey:	JLNIANBOPCTTQD-GJNRJIMPSA-N
Formula:	C29H52O4
SMILES:	CCCCC=CCCCOC(=O)C=CC(=O)OCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	464.72

Physical Properties

Property code	Value	Unit	Source
gf	-114.10	kJ/mol	Joback Method
hf	-897.05	kJ/mol	Joback Method
hfus	76.84	kJ/mol	Joback Method
hvap	98.38	kJ/mol	Joback Method
log10ws	-9.39		Crippen Method
logp	8.637		Crippen Method
mvol	425.750	ml/mol	McGowan Method
pc	690.34	kPa	Joback Method
rinpol	3281.00		NIST Webbook
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tb	1023.82	K	Joback Method
tc	1270.20	K	Joback Method
tf	550.75	K	Joback Method
vc	1.667	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1483.21	J/molxK	1023.82	Joback Method
cpg	1505.71	J/molxK	1064.88	Joback Method
cpg	1526.52	J/molxK	1105.95	Joback Method
cpg	1545.76	J/molxK	1147.01	Joback Method
cpg	1563.57	J/molxK	1188.07	Joback Method
cpg	1580.07	J/molxK	1229.14	Joback Method
cpg	1595.38	J/molxK	1270.20	Joback Method
dvisc	0.0002376	Paxs	550.75	Joback Method

dvisc	0.0001018	Paxs	629.60	Joback Method
dvisc	0.0000526	Paxs	708.44	Joback Method
dvisc	0.0000311	Paxs	787.29	Joback Method
dvisc	0.0000202	Paxs	866.13	Joback Method
dvisc	0.0000141	Paxs	944.98	Joback Method
dvisc	0.0000104	Paxs	1023.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348949&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
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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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