

Fumaric acid, heptyl tetradec-3-enyl ester

Inchi:	InChI=1S/C25H44O4/c1-3-5-7-9-10-11-12-13-14-15-17-19-23-29-25(27)21-20-24(26)28-
InchiKey:	SULMRNNJKVMXJE-SLIKNIJUSA-N
Formula:	C25H44O4
SMILES:	CCCCCCCCC=CCCOC(=O)C=CC(=O)OCCCCCCC
Mol. weight [g/mol]:	408.61

Physical Properties

Property code	Value	Unit	Source
gf	-147.78	kJ/mol	Joback Method
hf	-814.49	kJ/mol	Joback Method
hfus	66.48	kJ/mol	Joback Method
hvap	89.47	kJ/mol	Joback Method
log10ws	-7.72		Crippen Method
logp	7.076		Crippen Method
mvol	369.390	ml/mol	McGowan Method
pc	853.96	kPa	Joback Method
rinpol	2886.00		NIST Webbook
rinpol	2886.00		NIST Webbook
tb	932.30	K	Joback Method
tc	1142.51	K	Joback Method
tf	505.67	K	Joback Method
vc	1.444	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1226.29	J/molxK	932.30	Joback Method
cpg	1312.29	J/molxK	1107.47	Joback Method
cpg	1297.32	J/molxK	1072.44	Joback Method
cpg	1281.31	J/molxK	1037.40	Joback Method
cpg	1264.18	J/molxK	1002.37	Joback Method
cpg	1245.86	J/molxK	967.33	Joback Method
cpg	1326.26	J/molxK	1142.51	Joback Method
dvisc	0.0000193	Paxs	932.30	Joback Method

dvisc	0.0000260	Paxs	861.20	Joback Method
dvisc	0.0000370	Paxs	790.09	Joback Method
dvisc	0.0000562	Paxs	718.99	Joback Method
dvisc	0.0000938	Paxs	647.88	Joback Method
dvisc	0.0001776	Paxs	576.77	Joback Method
dvisc	0.0004022	Paxs	505.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348838&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
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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