

Fumaric acid, heptadecyl 3-methylbut-2-yl ester

Inchi:	InChI=1S/C26H48O4/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-22-29-25(27)20-21-2
InchiKey:	RBBNMCLKAABKCJ-QZQOTICOSA-N
Formula:	C26H48O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)C=CC(=O)OC(C)C(C)C
Mol. weight [g/mol]:	424.66

Physical Properties

Property code	Value	Unit	Source
gf	-224.46	kJ/mol	Joback Method
hf	-962.91	kJ/mol	Joback Method
hfus	61.83	kJ/mol	Joback Method
hvap	90.96	kJ/mol	Joback Method
log10ws	-8.15		Crippen Method
logp	7.545		Crippen Method
mcvol	387.780	ml/mol	McGowan Method
pc	791.71	kPa	Joback Method
rinqol	2860.00		NIST Webbook
tb	950.14	K	Joback Method
tc	1166.06	K	Joback Method
tf	492.02	K	Joback Method
vc	1.508	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1318.29	J/molxK	950.14	Joback Method
cpg	1406.15	J/molxK	1130.08	Joback Method
cpg	1391.34	J/molxK	1094.09	Joback Method
cpg	1375.21	J/molxK	1058.10	Joback Method
cpg	1357.70	J/molxK	1022.11	Joback Method
cpg	1338.75	J/molxK	986.13	Joback Method
cpg	1419.70	J/molxK	1166.06	Joback Method
dvisc	0.0000157	Paxs	950.14	Joback Method
dvisc	0.0000218	Paxs	873.79	Joback Method

dvisc	0.0000322	Paxs	797.43	Joback Method
dvisc	0.0000515	Paxs	721.08	Joback Method
dvisc	0.0000922	Paxs	644.73	Joback Method
dvisc	0.0001932	Paxs	568.37	Joback Method
dvisc	0.0005087	Paxs	492.02	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348088&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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